C-H Bond Activation by Unsymmetrical 2-(*N*-Arylimino)-pyrrolide Pt complexes: Geometric Effects on Reactivity

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Supporting Information

I. Preparation and NMR data of new complexes

General Details. All experiments were preformed in inert atmosphere using standard gloveboxe or Schlenk line techniques. Acetonitrile, benzene, hexamethyldisiloxane and methylene chloride were dried over 4Å molecular sieves. Diethyl ether, hexanes and toluene were dried by passage through cylinders of activated alumina and 4Å molecular sieves. C_6D_6 was dried and stored over 4Å molecular sieves. 2-iminopyrroles,[1] $[(SMe_2)PtMe_2]_2$[2] and $(SMe_2)_2Pt(Me)Cl$[2] were prepared via literature methods. The lithium salts of 2-iminopyrroles were prepared by reaction with BuLi in hexanes and isolated by suction filtration in the glovebox.

Complexes ***cis*-2a-c** were synthesized via the following method: $[(SMe_2)PtMe_2]_2$ and 2 molar equivalents of 2-iminopyrrole were dissolved in benzene in scintillation vials. The resulting yellow, homogenous solutions was stirred for 2-3 days at room temperature. The solvent was removed and the yellow solids were recrystallized from cold CH_2Cl_2 solutions layered with hexamethyldisiloxane in moderate yields.

Complexes ***trans*-2a,b,d** were prepared via the following method: *trans*-$(SMe_2)_2Pt(Me)Cl$ was suspended in 6 mL Et_2O in a scintillation vial. One molar equivalent of the lithium salt of 2-

[1] a) Miller, R.; Olsson, K. *Acta Chem. Scandia., B* **1981**, *35*, 303. a) Olsson, K.; Pernemalm, P.A. *Acta Chem. Scandia., B* **1979**, *33*, 125.
[2] Scott, J.D.; Puddephatt, R.J. *Organometallics* **1983**, *2*, 1643-1648.

iminopyrrole was added in portions to the suspension at room temperature over several minutes. The dark yellow mixture was allowed to stir overnight. The mixture was then filtered through a plug of celite and the filtrate reduced to a dark yellow solid under vacuum. The target compounds could not be separated from the *cis* isomers; however, ^{1}H NMR spectroscopic analysis was used for positive identification.

(SMe$_2$)Pt[iminopyrrolide(*p*-C$_6$H$_4$OMe)]Me (*cis*-2b). (103 mg, 63%). ^{1}H NMR (C_6D_6); δ 7.62 (broad s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 18 Hz, 1 H, pyrrole), 7.61 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 31 Hz, 1 H, C(H)=N), 6.98 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 1 Hz, 1 H, pyrrole), 6.84 (m, 2 H, C$_6$*H$_4$*OMe), 6.72 (m, 2 H, C$_6$*H$_4$*OMe), 6.51 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 2 Hz, 1 H, pyrrole), 3.28 (s, 3 H, OMe), 1.52 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 51 Hz, 6 H, SMe$_2$), 1.31 (s with ^{195}Pt satellites, $^{2}J_{Pt–H}$ = 79 Hz, 3 H, Pt–Me). ^{13}C NMR (C_6D_6); δ 158.6 (s with ^{195}Pt satellites, $J_{Pt–C}$ = 24 Hz), 133.6 (s with ^{195}Pt satellites, $J_{Pt–C}$ = 92 Hz), 123.9 (s), 118.8 (s with ^{195}Pt satellites, $J_{Pt–C}$ = 34 Hz), 113.9 (s), 111.1 (s with ^{195}Pt satellites, $J_{Pt–C}$ = 51 Hz), 54.7 (s, OMe), 20.3 (s with ^{195}Pt satellites, $^{2}J_{Pt–C}$ = 10.7 Hz, SMe$_2$), -17.3 (s with ^{195}Pt satellites, $^{1}J_{Pt–C}$ = 733 Hz), quaternary carbons not observed.

(SMe$_2$)Pt[iminopyrrolide(*p*-C$_6$H$_4$OMe)]Me (*trans*-2b). ^{1}H NMR (C_6D_6); δ 7.36 (s with ^{195}Pt shoulders, 1 H, pyrroleC(H)=N), 7.03 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 1 Hz, 1 H, pyrrole), 6.99 (m, 2 H, C$_6$*H$_4$*OMe), 6.68 (m, 2 H, C$_6$*H$_4$*OMe), 3.24 (s, 3 H, OMe), 1.73 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 57 Hz, 6 H, SMe$_2$), 0.74 (s with ^{195}Pt satellites, $^{2}J_{Pt–H}$ = 73 Hz, 3 H, Pt–Me), one pyrrole H obscured by other aromatic resonances.

(SMe$_2$)Pt[iminopyrrolide(*p*-C$_6$H$_4$CF$_3$)]Me (*cis*-2a). (107 mg, 64%). ^{1}H NMR (C_6D_6); δ 7.57 (m with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 21 Hz, 1 H, pyrrole), 7.39 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 31 Hz, 1 H, C(H)=N), 6.84 (d, $^{3}J_{H–H}$ = 8 Hz, 2 H, C$_6$*H$_4$*CF$_3$), 7.00 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 1 Hz, 1 H, pyrrole), 6.69 (d, $^{3}J_{H–H}$ = 8 Hz, 2 H, C$_6$*H$_4$*CF$_3$), 6.55 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 2 Hz, 1 H, pyrrole), 1.43 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 51 Hz, 6 H, SMe$_2$), 1.26 (s with ^{195}Pt satellites, $^{2}J_{Pt–H}$ = 80 Hz, 3 H, Pt–Me). ^{13}C NMR (C_6D_6); δ 158.6 (s with ^{195}Pt satellites, $J_{Pt–C}$ = 23 Hz), 135.0 (s with ^{195}Pt satellites, $J_{Pt–C}$ = 92 Hz), 125.9 (q, $^{3}J_{C–F}$ = 3.8 Hz, C *ortho* to CF$_3$), 123.4 (s, C *meta* to CF$_3$), 120.5 (s with ^{195}Pt satellites, $J_{Pt–C}$ = 33 Hz), 112.1 (s with ^{195}Pt satellites, $J_{Pt–C}$ = 52

Hz), 20.1 (s with ^{195}Pt satellites, $^{2}J_{Pt–C}$ = 10.5 Hz, SMe_2), -17.1 (s with ^{195}Pt satellites, $^{1}J_{Pt–C}$ = 739 Hz), quaternary carbons not observed.

(SMe_2)Pt[iminopyrrolide(*p*-$C_6H_4CF_3$)]Me (*trans*-2a). ^{1}H NMR (C_6D_6); δ 7.32 (m with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 21 Hz, 1 H, pyrrole), 7.18 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 31 Hz, 1 H, C(H)=N), 7.27 (d, $^{3}J_{H–H}$ = 8 Hz, 2 H, $C_6H_4CF_3$), 7.03 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 1 Hz, 1 H, pyrrole), 6.83 (d, $^{3}J_{H–H}$ = 8 Hz, 2 H, $C_6H_4CF_3$), 6.70 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 2 Hz, 1 H, pyrrole), 1.68 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 58 Hz, 6 H, SMe_2), 0.58 (s with ^{195}Pt satellites, $^{2}J_{Pt–H}$ = 73 Hz, 3 H, Pt–Me).

(SMe_2)Pt[iminopyrrolide(3,5-$(CF_3)_2C_6H_3$)]Me (*cis*-2c). (77 mg, 51%). ^{1}H NMR (C_6D_6); δ 7.56 (s, 2 H, C_6H_3), 7.53 (m, 1 H, pyrrole), 7.14 (s, 1 H, C_6H_3), 7.11 (s with ^{195}Pt satellites, $J_{Pt–H}$ = 35 Hz, 1 H, C(H)=N), 6.70 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 1 Hz, 1 H, pyrrole), 6.53 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 2 Hz, 1 H, pyrrole), 1.45 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 52 Hz, 6 H, SMe_2), 1.22 (s with ^{195}Pt satellites, $^{2}J_{Pt–H}$ = 81 Hz, 3 H, Pt–Me). Anal. Calc for $C_{16}H_{16}F_6N_2PtS$: C, 33.28; H, 2.79; N, 4.85. Found: C, 33.41; H, 2.78; N, 4.76.

(SMe_2)Pt[iminopyrrolide(2,6-$^{i}Pr_2C_6H_3$)]Me (*trans*-2d). ^{1}H NMR (C_6D_6); δ 7.51 (s, ^{195}Pt satellites obscured by other resonances, 1 H, C(H)=N), 7.32 (m, ^{195}Pt satellites obscured by other resonances, 1 H, pyrrole), 7.15 (m, 3 H, 2,6-Dipp), 7.04 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 1 Hz, 1 H, pyrrole), 6.72 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 1 Hz, 1 H, pyrrole), 3.62 (sept, $^{3}J_{H–H}$ = 7 Hz, 2 H, $CH(CH_3)_2$), 1.71 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 58 Hz, 6 H, SMe_2), 1.33 (d , $^{3}J_{H–H}$ = 7 Hz, 6 H, $CH(CH_3)_2$), 1.02 (d , $^{3}J_{H–H}$ = 7 Hz, 6 H, $CH(CH_3)_2$) 0.42 (s with ^{195}Pt satellites, $^{2}J_{Pt–H}$ = 73 Hz, 3 H, Pt-CH_3).

Complexes ***cis*-3a,b-d_5** were prepared via thermolysis of C_6D_6 solutions of ***cis*-2a,b** (0.017 mmol compound in 0.6 mL solvent in a J. Young NMR tube).

(SMe_2)Pt[iminopyrrolide(*p*-C_6H_4OMe)](Ph-d_5) (*cis*-3b-d_5). ^{1}H NMR (C_6D_6); δ 7.47 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 32 Hz, 1 H, C(H)=N), 6.88 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 1 Hz, 1 H, pyrrole), 6.86 (m, 2 H, C_6H_4OMe), 6.73 (m, 2 H, C_6H_4OMe), 6.36 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 2 Hz, 1 H,

pyrrole), 3.28 (s, 3 H, OMe), 1.37 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 51 Hz, 6 H, SMe_2), one pyrrole H obscured by other aromatic resonances.

(SMe_2)Pt[iminopyrrolide(*p*-$C_6H_4CF_3$)](Ph-d_5) (*cis*-3a-d_5). ^{1}H NMR (C_6D_6); δ 7.34 (d, $^{3}J_{H–H}$ = 8 Hz, 2 H, $C_6H_4CF_3$), 7.25 (s, ^{195}Pt satellites obscured by other signals, C(H)=N), 6.89 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 1 Hz, 1 H, pyrrole), 6.78 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 24 Hz, 1 H, pyrrole), 6.72 (d, $^{3}J_{H–H}$ = 8 Hz, 2 H, $C_6H_4CF_3$), 6.32 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 2 Hz, 1 H, pyrrole), 1.28 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 52 Hz, 6 H, SMe_2).

Complexes ***trans*-3d, 3e** were synthesized via the following method: $[(SMe_2)PtMe_2]_2$ and 2 molar equivalents of 2-iminopyrrole were dissolved in benzene in a Schlenk flask. The resulting yellow, homogenous solution was stirred overnight at room temperature. The solvent was removed and the yellow solids were recrystallized from cold toluene solutions in moderate yields.

(SMe_2)Pt[iminopyrrolide(2,6-$^{i}Pr_2C_6H_3$)]Ph (*trans*-3d). (0.25 g, 50%) ^{1}H NMR (C_6D_6); δ 7.51 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 83 Hz, 1 H, C(H)=N), 7.33 (dd, $^{3}J_{H–H}$ = 8 Hz, $^{4}J_{H–H}$ = 1 Hz, 2 H, *o*-H of Pt-Ph), 7.32 (m with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 25 Hz, 1 H, pyrrole), 7.00 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 1 Hz, 1 H, pyrrole), 6.88 (m, 3 H, $^{i}Pr_2C_6H_3$), 6.87 (m, 2 H, *m*-H of Pt-Ph), 6.76 (tt, $^{3}J_{H–H}$ = 7 Hz, $^{4}J_{H–H}$ = 2 Hz, 1 H, *p*-H of Pt-Ph), 6.68 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 2 Hz, 1 H, pyrrole), 1.52 (s with ^{195}Pt satellites, $^{3}J_{Pt–H}$ = 58 Hz, 6 H, SMe_2), 1.31 (d , $^{3}J_{H–H}$ = 7 Hz, 6 H, $CH(CH_3)_2$), 0.97 (d , $^{3}J_{H–H}$ = 7 Hz, 6 H, $CH(CH_3)_2$). ^{13}C NMR (C_6D_6); δ 163.3, 142.4, 137.3, 136.5 (s with ^{195}Pt satellites, $J_{Pt–C}$ = 41 Hz), 126.7, 126.6 (s with ^{195}Pt satellites, $J_{Pt–C}$ = 52 Hz), 122.7, 122.5, 120.0 (s with ^{195}Pt satellites, $J_{Pt–C}$ = 16), 112.8 (s with ^{195}Pt satellites, $J_{Pt–C}$ = 13), 27.7, 25.6, 22.23, 22.16 (SMe_2). Anal. Calc for $C_{25}H_{32}N_2PtS$: C, 51.09; H, 5.49; N, 4.77. Found: C, 50.67; H, 5.52; N, 4.71.

(SMe_2)Pt[iminopyrrolide(2,6-$Me_2C_6H_3$)]Ph (*trans*-3e). (0.21 g, 46%) ^{1}H NMR (C_6D_6); δ 7.32 (dd, $^{3}J_{H–H}$ = 8 Hz, $^{4}J_{H–H}$ = 1 Hz, 2 H, *o*-H of Pt-Ph), 7.30 (m with ^{195}Pt shoulders, 1 H, pyrrole), 6.96 (dd, $^{3}J_{H–H}$ = 4 Hz, $^{4}J_{H–H}$ = 1 Hz, 1 H, pyrrole), 6.90 (s ^{195}Pt satellites obscured by other resonances, 1 H, C(H)=N), 6.71 (m, 3 H, $^{i}Pr_2C_6H_3$), 6.76-6.88 (m, 3 H, *m,p*-H of Pt-Ph), 6.69

(dd, $^3J_{H-H}$ = 4 Hz, $^4J_{H-H}$ = 2 Hz, 1 H, pyrrole), 2.24 (s, 6 H, *Me*$_2$Ph), 1.50 (s with ^{195}Pt satellites, $^3J_{Pt-H}$ = 57 Hz, 6 H, SMe_2). Anal. Calc for $C_{21}H_{24}N_2PtS$: C, 47.45; H, 4.55; N, 5.27. Found: C, 47.16; H, 4.59; N, 5.32.

(NCCH$_3$)Pt[iminopyrrolide(2,6-^{i}Pr$_2$C$_6$H$_3$)]Me (*cis*-5d). $[(SMe_2)PtMe_2]_2$ (0.14 mg, 0.24 mmol) and 2 molar equivalents of 2-[N-(2,6-^{i}Pr$_2$C$_6$H$_3$)-imino]pyrrole (0.12 g, 0.48 mmol) were dissolved in acetonitrile in a Schlenk flask. The resulting yellow, homogenous solution was stirred for three days at room temperature. The solvent was removed and the yellow solids were recrystallized from cold toluene (0.24 g, 54%). ^{1}H NMR (C_6D_6); δ 7.62 (s with ^{195}Pt satellites, $^3J_{Pt-H}$ = 35 Hz, 1 H, C(H)=N), 7.53 (m, 1 H, pyrrole), 7.00 (m, 3 H, C_6H_3), 6.95 (dd, $^3J_{H-H}$ = 4 Hz, $^4J_{H-H}$ = 1 Hz, 1 H, pyrrole), 6.47 (dd, $^3J_{H-H}$ = 4 Hz, $^4J_{H-H}$ = 1 Hz, 1 H, pyrrole), 3.62 (sept, $^3J_{H-H}$ = 7 Hz, 2 H, C*H*$(CH_3)_2$), 1.69 (s with ^{195}Pt satellites, $^2J_{Pt-H}$ = 79 Hz, 3 H, Pt-CH_3), 1.17 (d , $^3J_{H-H}$ = 7 Hz, 6 H, CH(C*H*$_3$)$_2$), 1.04 (d, $^3J_{H-H}$ = 7 Hz, 6 H, CH(C*H*$_3$)$_2$), 0.22 (s, 3 H, $NCCH_3$). Anal. Calc for $C_{16}H_{16}F_6N_2PtS$: C, 47.61; H, 5.39; N, 8.33. Found: C, 47.76; H, 5.44; N, 8.15.

[Iminopyrrole(*p*-C$_6$H$_4$OMe)](SMe$_2$)PtMe$_2$ adduct. ^{1}H NMR (C_6D_6); δ 13.9 (broad s, 1 H, N-H), 8.04 (s with ^{195}Pt satellites, $^3J_{Pt-H}$ = 49 Hz, 1 H, C(H)=N), 7.75 (m, 2 H, C_6H_4OMe), 6.66 (m, 2 H, C_6H_4OMe), 6.51 (m, 2 H, pyrrole), 6.10 (m, 1 H, pyrrole), 3.28 (s, 3 H, OMe), 1.63 (s with ^{195}Pt satellites, $^3J_{Pt-H}$ = 22 Hz, 6 H, SMe_2), 1.33 (two overlapping singlets with ^{195}Pt satellites, $^2J_{Pt-H}$ = 84 Hz, 6 H, Pt–Me). ^{13}C NMR (C_6D_6); δ 113.98 (s with ^{195}Pt satellites, $^2J_{Pt-C}$ = 41 Hz, SMe_2), 54.97 (OMe), 20.05 (two overlapping singlets with ^{195}Pt satellites, $^1J_{Pt-C}$ = 94 Hz, Pt–Me).

[Iminopyrrole(*p*-C$_6$H$_4$CF$_3$)](SMe$_2$)PtMe$_2$ adduct. ^{1}H NMR (C_6D_6); δ 13.8 (broad s, 1 H, N-H), 7.76 (s with ^{195}Pt satellites, $^3J_{Pt-H}$ = 48 Hz, 1 H, C(H)=N), 7.25 (s, 4 H, $C_6H_4CF_3$), 6.52 (m, 1 H, pyrrole), 6.47 (br s, 1 H, pyrrole), 6.07 (m, 1 H, pyrrole), 1.55 (s with ^{195}Pt satellites, $^3J_{Pt-H}$ = 23 Hz, 6 H, SMe_2), 1.28 (s with ^{195}Pt satellites, $^2J_{Pt-H}$ = 86 Hz, 3 H, Pt–Me), 1.23 (s with ^{195}Pt satellites, $^2J_{Pt-H}$ = 84 Hz, 3 H, Pt–Me).

Thermolysis of complexes 2a,b in C$_6$D$_6$. A mixture of *cis*/*trans*-**2a** or *cis*/*trans*-**2b** (0.021 mmol), formed via the metathesis of $(SMe_2)_2Pt(Me)Cl$ with the appropriate iminopyrrolide

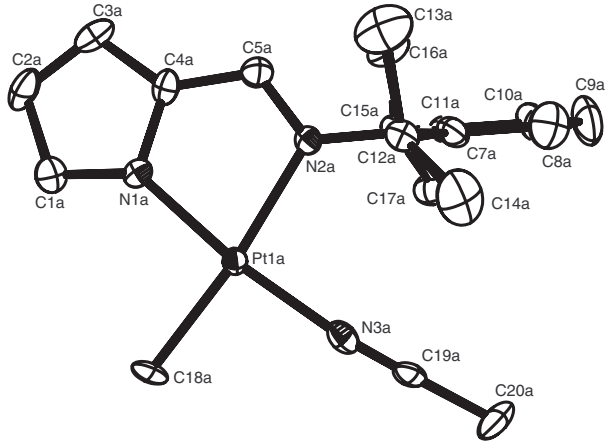
lithium salt, was dissolved in 600 μL in a J Young NMR tube. The sample was heated at 85 ºC and the progress of the reaction was monitored by ^{1}H NMR spectroscopy.

Reaction of complexes 2a,b with SMe_2-*d_6* in C_6D_6. Isolated *cis*-**2a** (14 mg, 0.032 mmol) or a 1:1 mixture of *cis*/*trans*-**2b** (14.8 mg, 0.031 mmol), formed via the metathesis of $(SMe_2)_2Pt(Me)Cl$ with the Li-**1b**, was dissolved in 600 μL in a J Young NMR tube. SMe_2-*d_6* (4.5 μL, 0.062 mmol) was added to the tube via microliter syringe. The sample was allowed to react at room temperature and the progress of the reaction was monitored by ^{1}H NMR spectroscopy.

II. Crystal Structure Data

1. (NCCH$_3$)Pt[iminopyrrolide(2,6-^{i}Pr$_2$C$_6$H$_3$)]Me (*cis*-5d)

Contents



$C_{20}H_{24}N_3Pt$

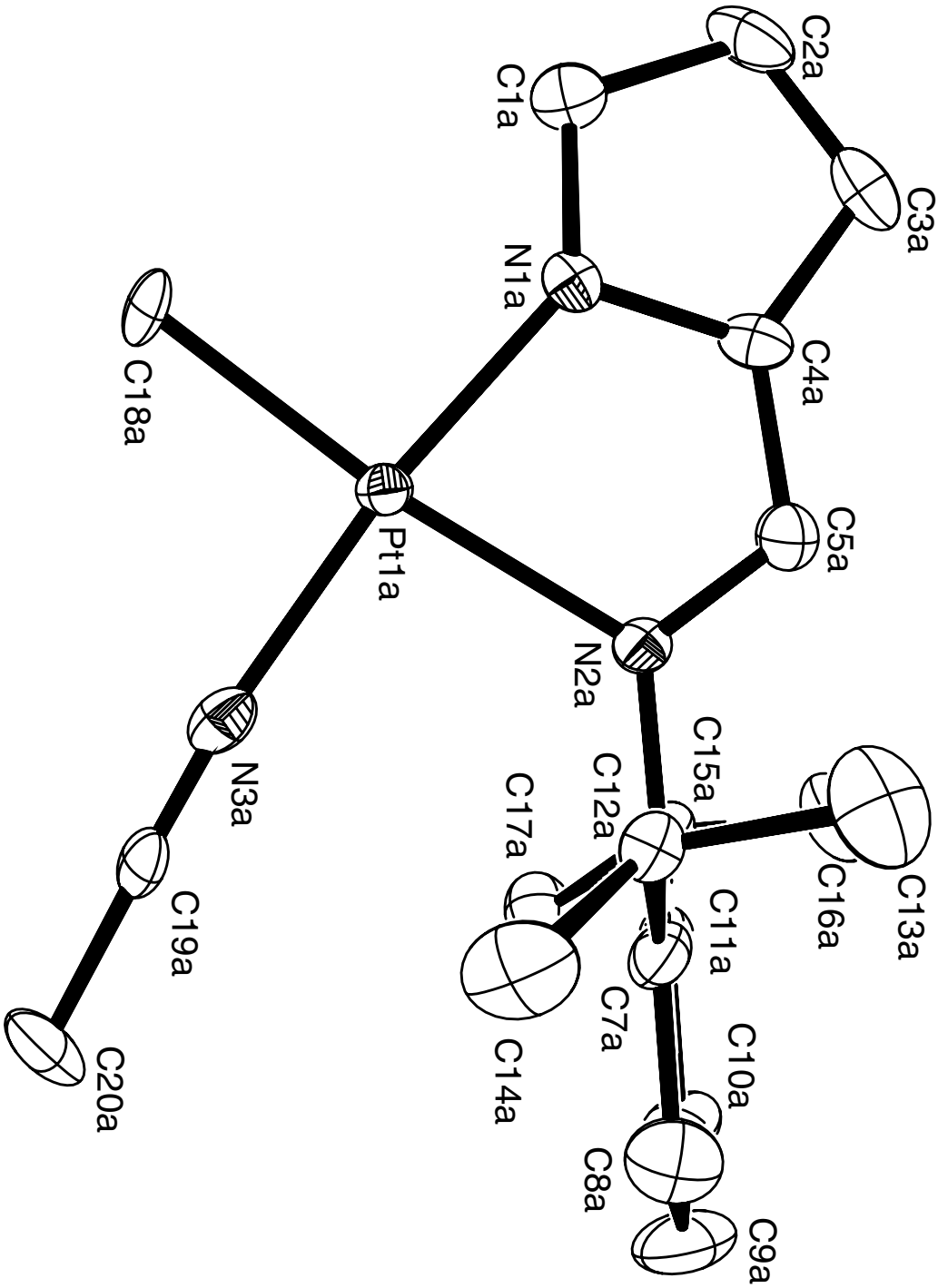


Figure 1. Labeled ORTEP-3[1] view of *cis*-5d (a) with 60% probability ellipsoids, without hydrogens.

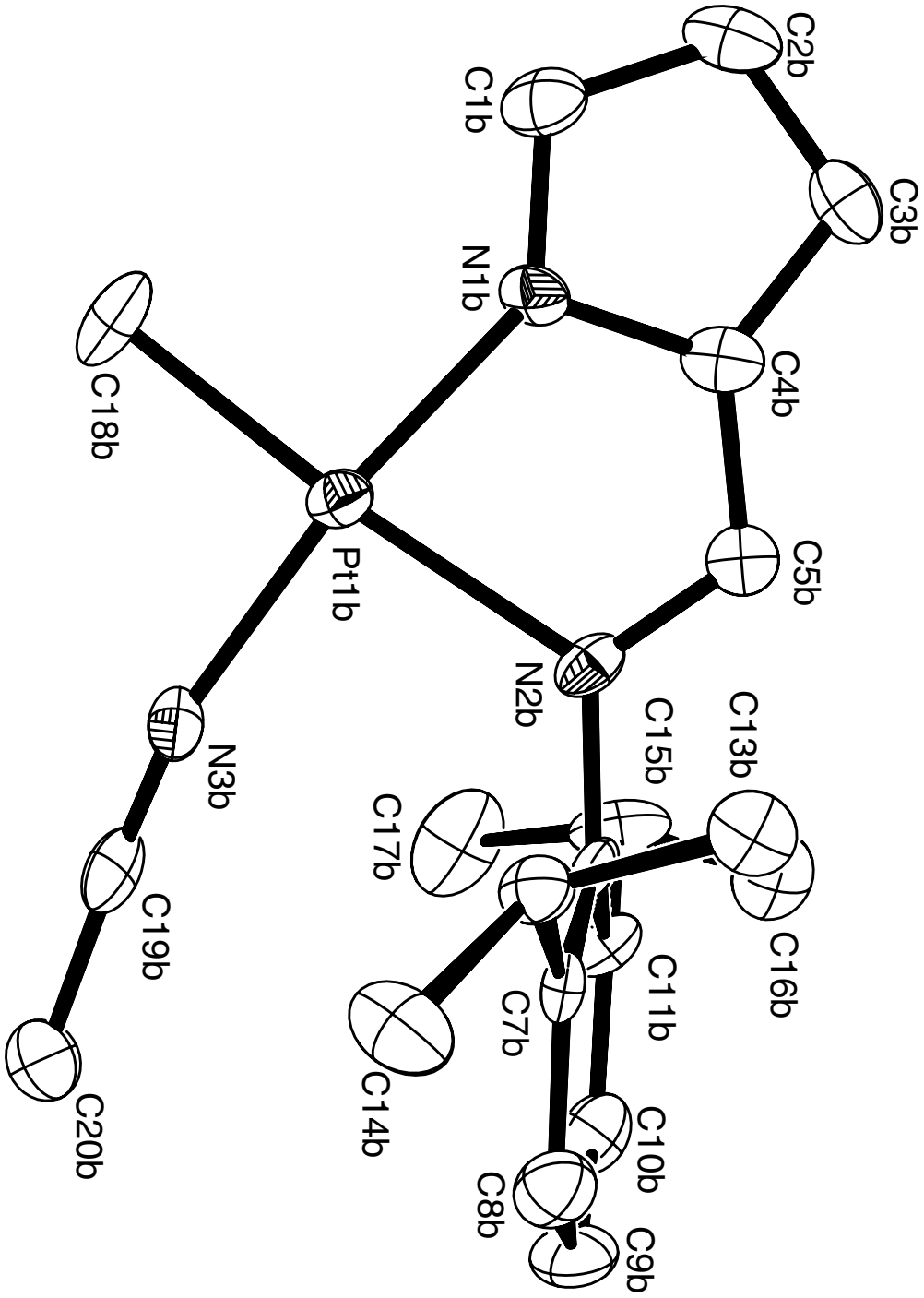


Figure 2. Labeled ORTEP-3[1] view of *cis*-5d (b) with 60% probability ellipsoids, without hydrogens.

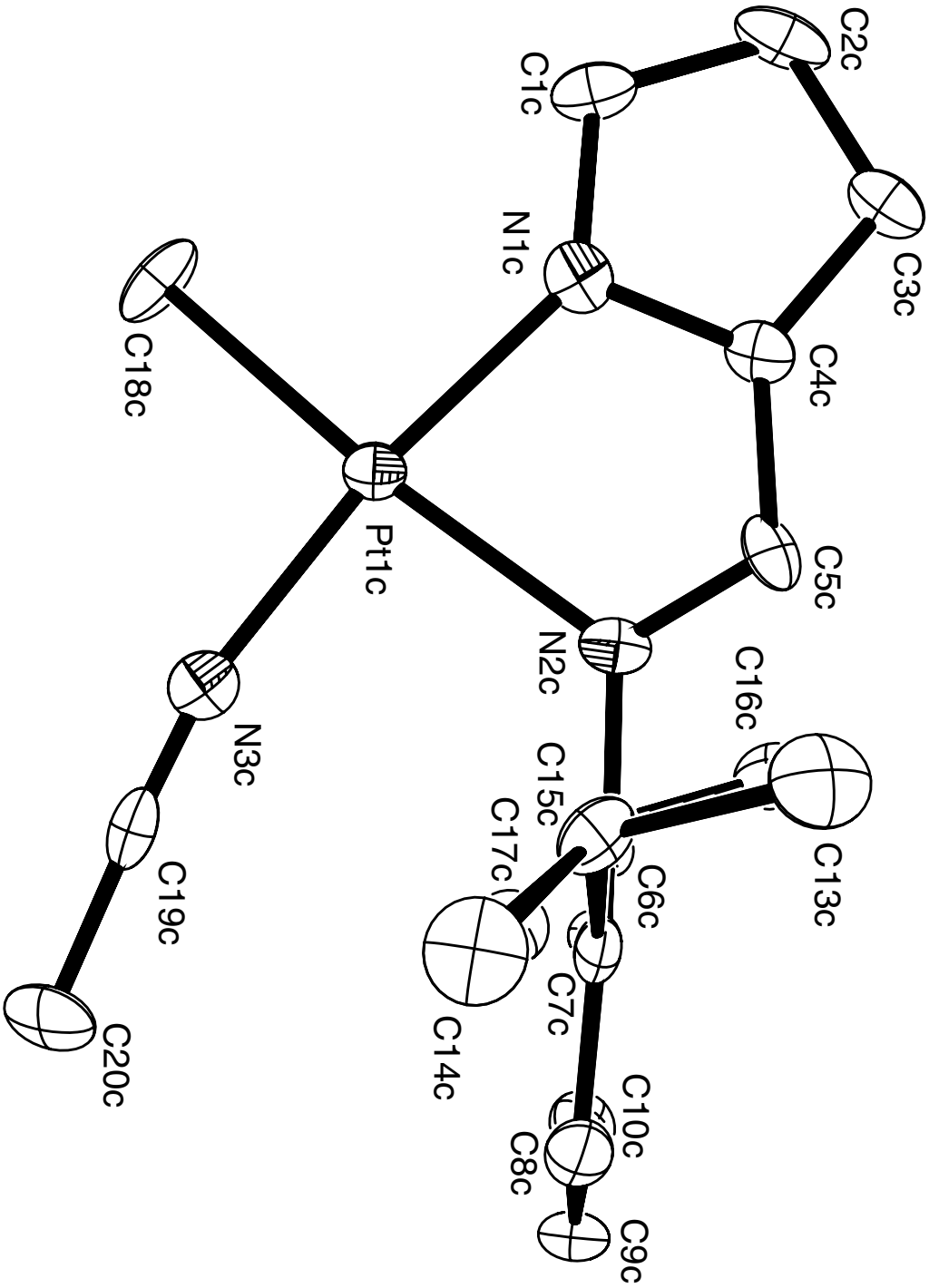


Figure 3. Labeled ORTEP-3[1] view of *cis*-5d (c) with 60% probability ellipsoids, without hydrogens.

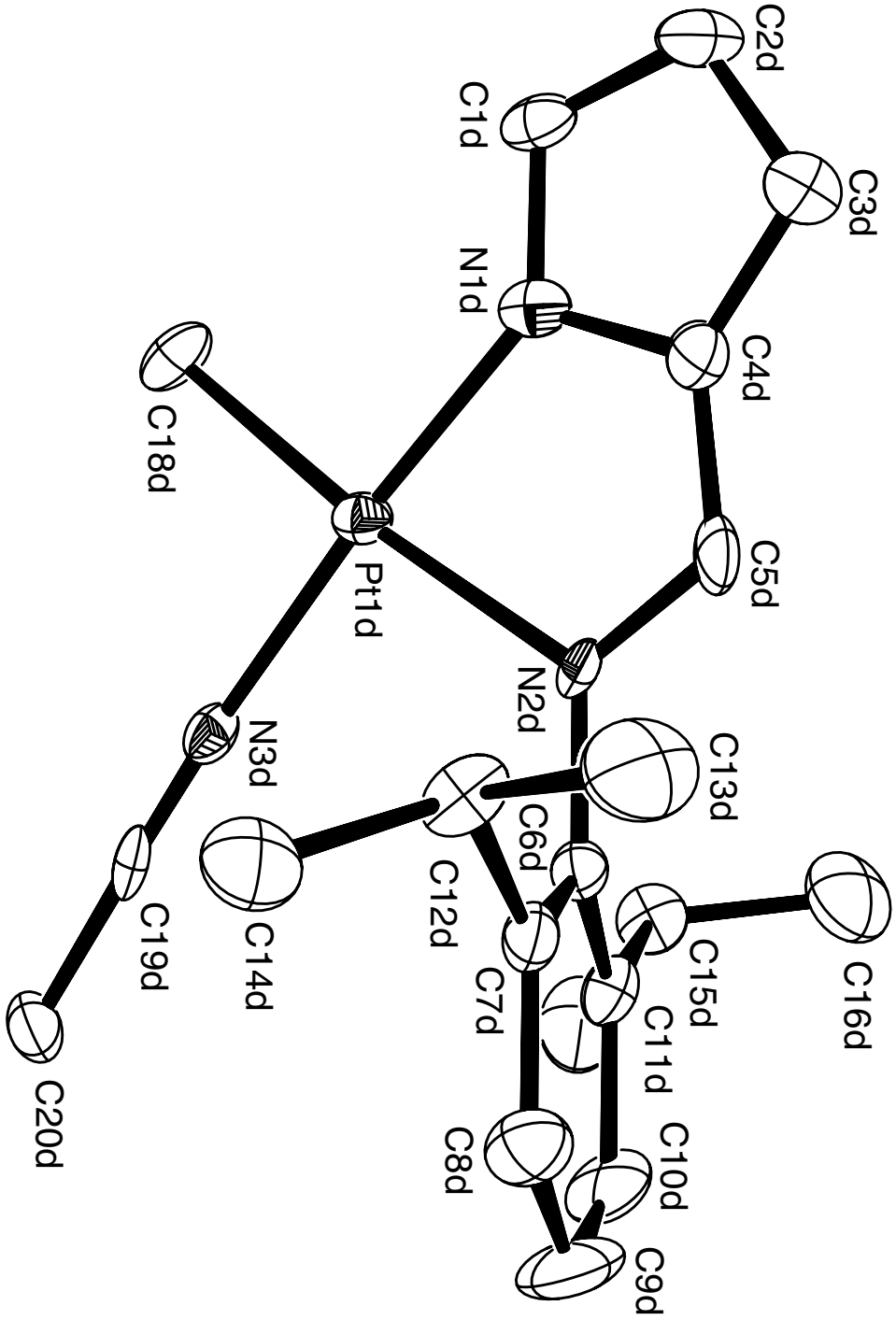


Figure 4. Labeled ORTEP-3[1] view of *cis*-5d (d) with 60% probability ellipsoids, without hydrogens.

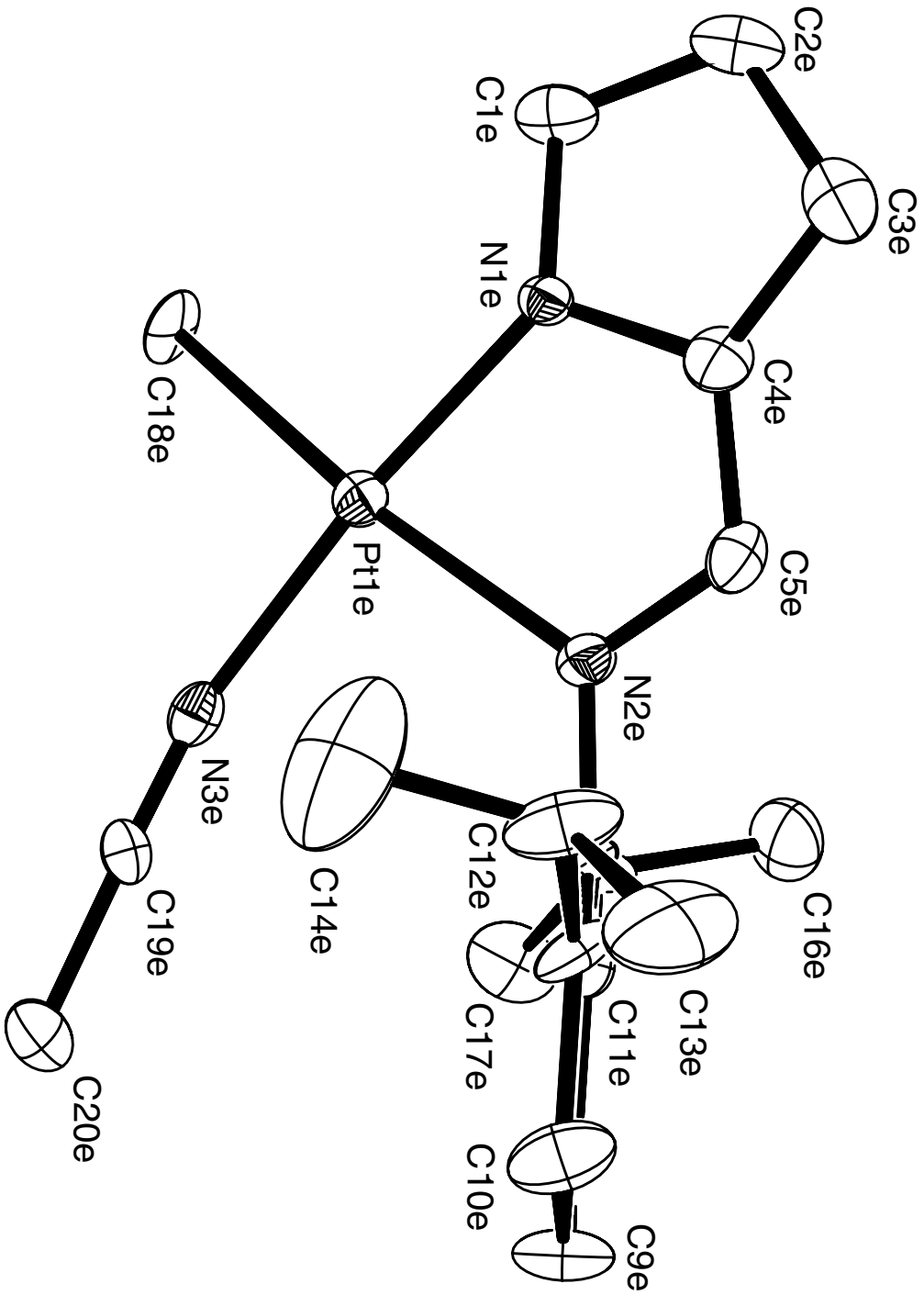


Figure 5. Labeled ORTEP-3[1] view of *cis*-5d (e) with 60% probability ellipsoids, without hydrogens.

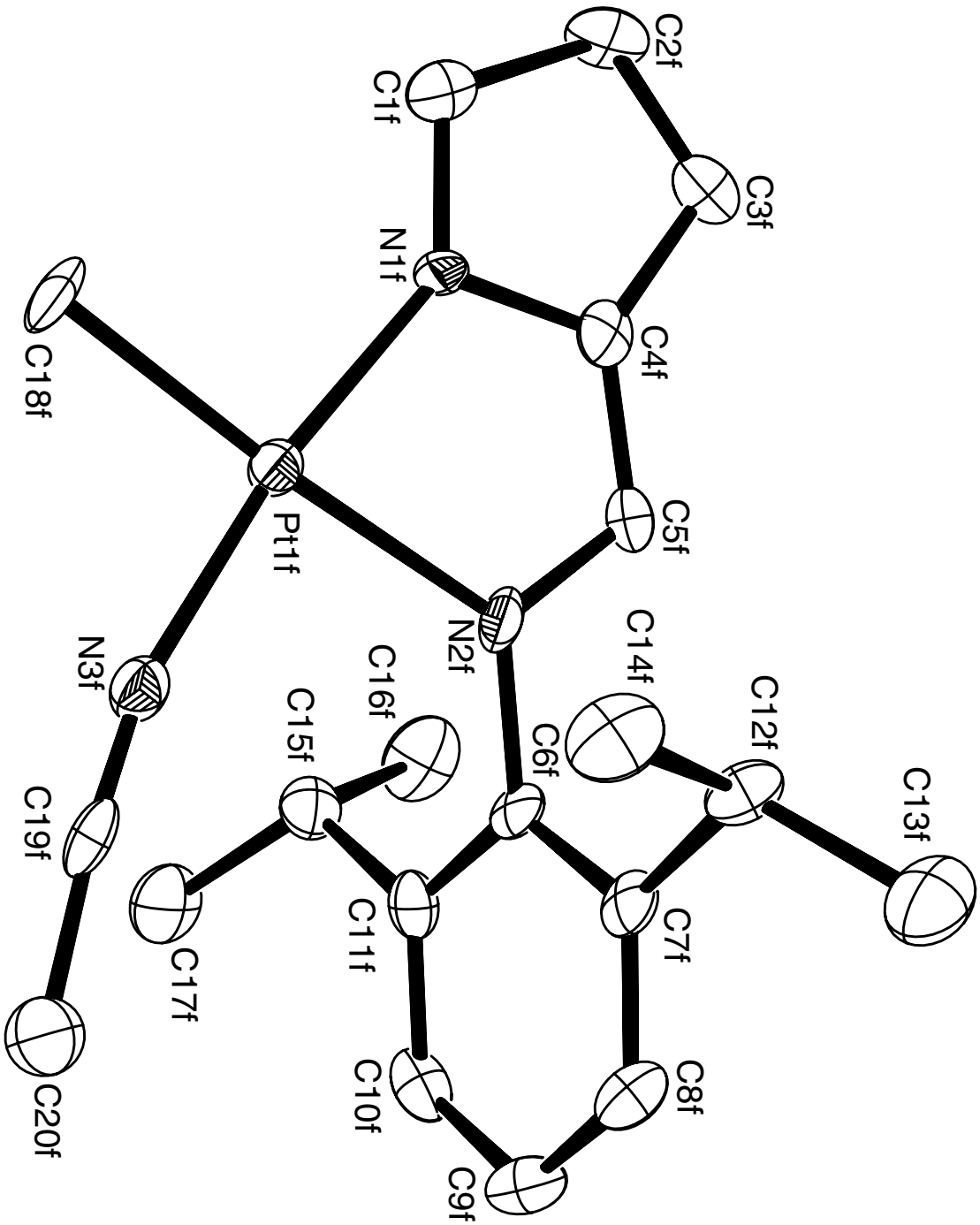


Figure 6. Labeled ORTEP-3[1] view of *cis*-5d (f) with 60% probability ellipsoids, without hydrogens.

Table 1. Crystal Data and Structure Analysis Details for ***cis*-5d**.

Empirical formula	$C_{20}H_{24}N_3Pt$	
Formula weight	501.51	
Crystallization solvent	toluene	
Crystal shape	rhombic	
Crystal color	pale yellow	
Crystal size	0.15 x 0.16 x 0.24 mm	
Data Collection		
Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000 ccd	
Wavelength	0.71073 Å MoKα	
Data collection temperature	98 K	
Theta range for 6677 reflections used in lattice determination	2.4 to 28.0°	
Unit cell dimensions	a = 24.0988(18) Å	α= 90°
	b = 11.5512(9) Å	β= 90.917(1)°
	c = 42.783(3) Å	γ = 90°
Volume	11908.0(15) $Å^3$	
Z	24	
Crystal system	monoclinic	
Space group	$P2_1/c$ (# 14)	
Density (calculated)	1.678 g/cm^3	
F(000)	5832	
Theta range for data collection	1.69 to 28.68°	
Completeness to theta = 28.68°	93.4%	
Index ranges	$-32 \le h \le 30$, $-15 \le k \le 14$, $-57 \le l \le 57$	
Data collection scan type	ω scans at 5 fixed ϕ values	
Reflections collected	175667	
Independent reflections	28704 [R_{int}= 0.0956]	
Reflections > 2σ(I)	20577	
Average σ(I)/(net I)	0.0734	
Absorption coefficient	7.075 mm^{-1}	
Absorption correction	integration	
Max. and min. transmission	0.462 and 0.167	
Number of standards	first scans recollected at end of runs	
Decay of standards	within counting statistics	
Structure Solution and Refinement		
Primary solution method	Patterson map	
Secondary solution method	difference map	
Hydrogen placement	calculated	
Refinement method	full-matrix least-squares on F^2	
Data / restraints / parameters	28704 / 0 / 1327	
Treatment of hydrogen atoms	calculated coordinates, rotated methyl groups, fixed U_{iso} at 120% of U_{eq} of attached atom	
Goodness-of-fit on F^2	1.306	
Final R indices [I>2σ(I), 20577 reflections]	R1 = 0.0442, wR2 = 0.0694	

Table 1. Crystal Data and Structure Analysis Details for ***cis*-5d**.

R indices (all data)	R1 = 0.0720, wR2 = 0.0724
Type of weighting scheme used	sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.005
Average shift/error	0.000
Largest diff. peak and hole	2.50 and -3.28 e·Å^{-3}

Table 1. Crystal Data and Structure Analysis Details for ***cis*-5d**.

	Programs Used
Cell refinement	Bruker SAINT v6.02
Data collection	Bruker SMART v5.606
Data reduction	Bruker SAINT v6.02
Structure solution	SHELXS-97 (Sheldrick, 1990)
Structure refinement	SHELXL-97 (Sheldrick, 1997)

Special Refinement Details

A small fragment was cut from a pale-yellow crystal and mounted on a glass fiber with Paratone-N oil. Five runs of data were collected with 15 second long, –0.30° wide ω–scans at five values of φ (0, 72, 144, 216, and 288°) with the detector 5 cm (nominal) distant at a θ of -28° using SMART v5.606. The initial cell for data reduction was calculated from just under 1000 reflections chosen from throughout the data frames. For data processing with SAINT v6.02, all defaults were used, except: a fixed box size of 1.8 x 1.8 x 0.7 was used, periodic orientation matrix updating was disabled, the instrument error was set to zero, no Laue class integration restraints were used, and for the post-integration global least squares refinement, no constraints were applied. The faces of the crystal were indexed, and a gaussian face-centered absorption correction was applied with XPREP v6.09 beta. No decay correction was needed. Using SADABS v2.02 beta did not improve refinement.

Two outlier reflections (4 1 0 and 1 1 32) were omitted from the final processed dataset; 4777 reflections were rejected, with 30 space group-absence violations and 94 inconsistent equivalents. Refinement of F^2 was against all reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement.

There are six molecules in the asymmetric unit. The conformations of the molecules differ primarily in the orientations of the isopropyl groups. Hydrogen atoms were placed at calculated positions with U_{iso}'s set at 120% of the U_{eq}'s of the attached atoms; the methyl groups were allowed to rotate. There are a number of large peaks in the final difference map; the four larger than |2| e·Å^{-3} are 2.50 (0.07Å from Pt1D), -3.28 (1.33Å from Pt1C), -2.99 (0.89Å from Pt1A), and -2.69 (1.15Å from Pt1B). Sixteen of the 20 largest peaks (all > |1| e·Å^{-3}) are near Pt atoms with one each near C18D and C11D and two near H3D. Almost all of the most disagreeable reflections have $Fo^2 > Fc^2$, perhaps indicating some twinning. However no pattern to these reflections could be discerned.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for ***cis*-5d**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Molecule *cis*-**5d (a)**

	x	y	z	U_{eq}
Pt1A	78(1)	6212(1)	1283(1)	12(1)
N1A	679(2)	7369(4)	1230(1)	13(1)
N2A	784(2)	5131(4)	1300(1)	13(1)
N3A	-448(2)	4916(5)	1317(1)	18(1)
C1A	721(3)	8504(6)	1174(1)	19(2)
C2A	1279(3)	8776(6)	1126(2)	26(2)
C3A	1577(3)	7793(6)	1158(2)	23(2)
C4A	1202(3)	6910(5)	1217(1)	16(1)
C5A	1239(3)	5707(6)	1264(2)	20(2)
C6A	782(2)	3881(5)	1328(1)	14(1)
C7A	727(2)	3394(6)	1625(2)	18(1)
C8A	714(3)	2203(6)	1643(2)	29(2)
C9A	747(3)	1527(6)	1380(2)	34(2)
C10A	789(3)	2027(6)	1088(2)	29(2)
C11A	802(2)	3216(6)	1053(1)	17(1)
C12A	705(2)	4133(6)	1915(2)	19(1)
C13A	1287(3)	4288(7)	2057(2)	36(2)
C14A	323(3)	3644(6)	2162(2)	32(2)
C15A	841(3)	3768(6)	735(1)	22(2)
C16A	1430(3)	3730(7)	613(2)	35(2)
C17A	447(3)	3221(6)	494(2)	31(2)
C18A	-558(2)	7430(6)	1265(2)	18(2)
C19A	-715(2)	4105(6)	1317(1)	16(1)
C20A	-1046(3)	3049(6)	1318(2)	27(2)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for ***cis*-5d**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Molecule *cis*-**5d (b)**

	x	y	z	U_{eq}
Pt1B	3763(1)	4072(1)	2062(1)	16(1)
N1B	3249(2)	4299(4)	1702(1)	17(1)
N2b	3168(2)	2768(4)	2151(1)	16(1)
N3B	4206(2)	3685(5)	2439(1)	18(1)
C1B	3203(3)	4968(6)	1445(2)	24(2)
C2b	2735(3)	4676(6)	1272(2)	25(2)
C3B	2473(3)	3790(6)	1429(2)	21(2)
C4B	2796(3)	3547(6)	1693(1)	18(2)
C5B	2771(3)	2762(5)	1944(1)	17(1)
C6B	3176(2)	2031(5)	2421(2)	15(1)
C7B	3502(2)	1011(5)	2417(1)	16(1)
C8B	3533(3)	353(6)	2685(2)	25(2)
C9B	3259(3)	705(6)	2952(2)	28(2)
C10B	2963(3)	1720(6)	2957(2)	25(2)
C11B	2913(3)	2404(6)	2689(2)	19(2)
C12b	3806(2)	666(6)	2121(1)	18(2)
C13B	3421(3)	51(6)	1887(2)	22(2)
C14B	4321(3)	-68(6)	2188(2)	28(2)
C15B	2602(3)	3560(6)	2702(2)	27(2)
C16B	2006(3)	3415(6)	2806(2)	34(2)
C17B	2907(3)	4404(6)	2914(2)	41(2)
C18B	4295(3)	5396(7)	1945(2)	35(2)
C19B	4387(3)	3302(6)	2661(2)	21(2)
C20B	4593(3)	2773(6)	2944(2)	29(2)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for ***cis*-5d**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Molecule *cis*-**5d (c)**

	x	y	z	U_{eq}
Pt1C	1180(1)	6532(1)	2875(1)	14(1)
N1C	1696(2)	6194(4)	3235(1)	17(1)
N2C	1801(2)	7797(4)	2801(1)	14(1)
N3C	760(2)	7006(5)	2503(1)	19(1)
C1C	1732(3)	5457(6)	3471(1)	18(2)
C2C	2209(3)	5672(6)	3648(1)	22(2)
C3C	2470(3)	6608(6)	3511(1)	18(2)
C4C	2153(3)	6929(5)	3253(1)	16(1)
C5C	2192(2)	7770(6)	3009(1)	17(2)
C6C	1803(2)	8600(6)	2543(1)	15(1)
C7C	2041(2)	8250(5)	2260(2)	17(1)
C8C	2005(2)	8998(6)	2008(1)	19(2)
C9C	1737(3)	10064(6)	2036(2)	23(2)
C10C	1491(3)	10376(6)	2315(2)	19(2)
C11C	1505(3)	9639(6)	2574(2)	18(2)
C12C	2311(2)	7064(6)	2231(2)	19(2)
C13C	2909(3)	7070(6)	2355(2)	29(2)
C14C	2290(3)	6595(6)	1903(2)	29(2)
C15C	1214(3)	9930(5)	2876(2)	20(2)
C16C	1618(3)	10389(6)	3124(2)	25(2)
C17C	736(3)	10810(6)	2825(2)	29(2)
C18C	602(3)	5285(6)	2994(2)	28(2)
C19C	595(3)	7413(6)	2278(2)	17(2)
C20C	411(3)	7955(6)	1986(1)	25(2)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for ***cis*-5d**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Molecule *cis*-**5d (d)**

	x	y	z	U_{eq}
Pt1D	4877(1)	4265(1)	3701(1)	14(1)
N1D	4252(2)	3135(4)	3711(1)	16(1)
N2D	4192(2)	5402(4)	3747(1)	15(1)
N3D	5441(2)	5489(5)	3704(1)	15(1)
C1D	4184(3)	1991(6)	3713(1)	19(2)
C2D	3634(3)	1706(6)	3755(2)	28(2)
C3D	3355(3)	2744(6)	3780(2)	27(2)
C4D	3735(3)	3618(6)	3752(2)	21(2)
C5D	3724(3)	4840(6)	3770(2)	20(2)
C6D	4217(2)	6633(5)	3795(1)	16(1)
C7D	4171(2)	7045(6)	4102(2)	17(1)
C8D	4204(3)	8238(6)	4142(2)	25(2)
C9D	4286(3)	8979(6)	3898(2)	37(2)
C10D	4349(3)	8554(6)	3602(2)	31(2)
C11D	4326(2)	7350(6)	3543(1)	17(1)
C12D	4122(3)	6270(6)	4384(1)	19(2)
C13D	3541(3)	6284(7)	4512(2)	39(2)
C14D	4549(3)	6570(6)	4636(2)	30(2)
C15D	4380(3)	6887(6)	3220(1)	22(2)
C16D	3826(3)	6856(7)	3049(2)	38(2)
C17D	4797(3)	7515(7)	3017(2)	38(2)
C18D	5484(3)	3022(6)	3668(2)	20(2)
C19D	5741(3)	6251(6)	3715(2)	18(2)
C20D	6119(3)	7231(6)	3720(2)	22(2)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for ***cis*-5d**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Molecule *cis*-**5d (e)**

	x	y	z	U_{eq}
Pt1E	3776(1)	4104(1)	5388(1)	14(1)
N1E	3289(2)	4462(4)	5742(1)	12(1)
N2E	3221(2)	2689(4)	5361(1)	15(1)
N3E	4170(2)	3625(4)	5006(1)	15(1)
C1E	3233(3)	5294(6)	5957(1)	20(2)
C2E	2759(3)	5073(6)	6140(2)	22(2)
C3E	2523(3)	4065(6)	6026(2)	24(2)
C4E	2856(2)	3683(5)	5783(2)	18(2)
C5E	2841(2)	2730(5)	5576(2)	18(2)
C6E	3220(3)	1773(5)	5132(2)	17(1)
C7E	2835(3)	1809(5)	4886(2)	19(2)
C8E	2882(3)	963(6)	4657(2)	28(2)
C9E	3288(3)	120(6)	4671(2)	26(2)
C10E	3672(3)	114(6)	4914(2)	21(2)
C11E	3648(2)	937(6)	5150(1)	17(1)
C12E	2404(3)	2770(6)	4860(2)	28(2)
C13E	1870(3)	2377(7)	4721(2)	41(2)
C14E	2635(3)	3783(7)	4700(3)	66(3)
C15E	4066(3)	933(6)	5427(1)	21(2)
C16E	3832(3)	266(7)	5701(2)	34(2)
C17E	4626(3)	457(7)	5346(2)	34(2)
C18E	4297(3)	5492(5)	5468(2)	19(2)
C19E	4305(3)	3226(6)	4780(2)	17(1)
C20E	4464(3)	2684(6)	4485(2)	26(2)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for ***cis*-5d**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Molecule *cis*-**5d (f)**

	x	y	z	U_{eq}
Pt1F	8822(1)	4141(1)	403(1)	15(1)
N1F	8320(2)	4542(4)	752(1)	15(1)
N2F	8265(2)	2726(4)	384(1)	17(1)
N3F	9223(2)	3616(5)	36(1)	18(1)
C1F	8256(3)	5422(6)	953(1)	18(2)
C2F	7774(3)	5228(6)	1127(1)	21(2)
C3F	7541(3)	4196(6)	1026(1)	19(2)
C4F	7881(2)	3783(5)	789(2)	17(2)
C5F	7872(2)	2804(5)	590(1)	15(1)
C6F	8279(2)	1796(5)	160(1)	15(1)
C7F	7900(2)	1799(5)	-97(2)	17(1)
C8F	7953(3)	940(6)	-319(2)	21(2)
C9F	8361(3)	101(6)	-299(2)	23(2)
C10F	8735(3)	125(5)	-47(2)	20(2)
C11F	8707(2)	965(6)	184(1)	17(1)
C12F	7472(3)	2771(5)	-134(2)	19(2)
C13F	6962(3)	2395(6)	-321(2)	32(2)
C14F	7738(3)	3835(6)	-281(2)	28(2)
C15F	9107(3)	966(6)	468(2)	21(2)
C16F	8845(3)	361(7)	749(2)	33(2)
C17F	9660(3)	443(7)	400(2)	32(2)
C18F	9338(3)	5545(6)	456(2)	24(2)
C19F	9371(3)	3181(6)	-186(2)	19(2)
C20F	9510(3)	2585(6)	-473(2)	26(2)

Table 3. Bond lengths [Å] for ***cis*-5d**.

Molecule *cis*-**5d (a)**	
Pt1A-N3A	1.969(6)
Pt1A-N1A	1.987(5)
Pt1A-C18A	2.081(6)
Pt1A-N2A	2.111(5)
N1A-C1A	1.336(8)
N1A-C4A	1.370(7)
N2A-C5A	1.292(7)
N2A-C6A	1.450(8)
N3A-C19A	1.136(8)
C1A-C2A	1.399(9)
C1A-H1A	0.9500
C2A-C3A	1.350(9)
C2A-H2A	0.9500
C3A-C4A	1.388(9)
C3A-H3A	0.9500
C4A-C5A	1.407(9)
C5A-H5A	0.9500
C6A-C7A	1.401(8)
C6A-C11A	1.404(8)
C7A-C8A	1.379(9)
C7A-C12A	1.508(9)
C8A-C9A	1.372(10)
C8A-H8A	0.9500
C9A-C10A	1.383(10)
C9A-H9A	0.9500
C10A-C11A	1.381(9)
C10A-H10A	0.9500
C11A-C15A	1.509(9)
C12A-C14A	1.520(9)
C12A-C13A	1.529(8)
C12A-H12A	1.0000
C13A-H13A	0.9800
C13A-H13B	0.9800
C13A-H13C	0.9800
C14A-H14A	0.9800
C14A-H14B	0.9800
C14A-H14C	0.9800
C15A-C16A	1.521(9)
C15A-C17A	1.526(8)
C15A-H15A	1.0000
C16A-H16A	0.9800
C16A-H16B	0.9800
C16A-H16C	0.9800
C17A-H17A	0.9800
C17A-H17B	0.9800
C17A-H17C	0.9800
C19A-C20A	1.458(9)
C20A-H20A	0.9800
C20A-H20B	0.9800
C20A-H20C	0.9800

Table 3. Bond lengths [Å] for ***cis*-5d**.

Molecule *cis*-**5d (b)**	
Pt1B-N3B	1.971(5)
Pt1B-N1B	1.977(5)
Pt1B-C18B	2.062(7)
Pt1B-N2b	2.118(5)
N1B-C1B	1.346(8)
N1B-C4B	1.394(8)
N2b-C5B	1.296(7)
N2b-C6B	1.435(8)
N3B-C19B	1.130(8)
C1B-C2b	1.382(8)
C1B-H1B	0.9500
C2b-C3B	1.382(9)
C2b-H2b	0.9500
C3B-C4B	1.388(8)
C3B-H3B	0.9500
C4B-C5B	1.406(9)
C5B-H5B	0.9500
C6B-C11B	1.387(9)
C6B-C7B	1.417(8)
C7B-C8B	1.377(9)
C7B-C12b	1.527(8)
C8B-C9B	1.392(9)
C8B-H8B	0.9500
C9B-C10B	1.373(9)
C9B-H9B	0.9500
C10B-C11B	1.396(9)
C10B-H10B	0.9500
C11B-C15B	1.532(9)
C12b-C14B	1.527(8)
C12b-C13B	1.528(8)
C12b-H12b	1.0000
C13B-H13D	0.9800
C13B-H13E	0.9800
C13B-H13F	0.9800
C14B-H14D	0.9800
C14B-H14E	0.9800
C14B-H14F	0.9800
C15B-C17B	1.515(9)
C15B-C16B	1.523(9)
C15B-H15B	1.0000
C16B-H16D	0.9800
C16B-H16E	0.9800
C16B-H16F	0.9800
C17B-H17D	0.9800
C17B-H17E	0.9800
C17B-H17F	0.9800
C19B-C20B	1.438(9)
C20B-H20D	0.9800
C20B-H20E	0.9800
C20B-H20F	0.9800

Table 3. Bond lengths [Å] for ***cis*-5d**.

Molecule *cis*-**5d (c)**	
Pt1C-N3C	1.951(5)
Pt1C-N1C	2.003(5)
Pt1C-C18C	2.073(6)
Pt1C-N2C	2.118(5)
N1C-C1C	1.323(8)
N1C-C4C	1.392(8)
N2C-C5C	1.290(7)
N2C-C6C	1.441(7)
N3C-C19C	1.136(8)
C1C-C2C	1.388(8)
C1C-H1C	0.9500
C2C-C3C	1.386(9)
C2C-H2C	0.9500
C3C-C4C	1.384(8)
C3C-H3C	0.9500
C4C-C5C	1.429(9)
C5C-H5C	0.9500
C6C-C7C	1.406(9)
C6C-C11C	1.406(9)
C7C-C8C	1.384(8)
C7C-C12C	1.523(9)
C8C-C9C	1.397(9)
C8C-H8C	0.9500
C9C-C10C	1.389(9)
C9C-H9C	0.9500
C10C-C11C	1.397(8)
C10C-H10C	0.9500
C11C-C15C	1.517(9)
C12C-C14C	1.504(9)
C12C-C13C	1.528(8)
C12C-H12C	1.0000
C13C-H13G	0.9800
C13C-H13H	0.9800
C13C-H13I	0.9800
C14C-H14G	0.9800
C14C-H14H	0.9800
C14C-H14I	0.9800
C15C-C16C	1.522(8)
C15C-C17C	1.550(8)
C15C-H15C	1.0000
C16C-H16G	0.9800
C16C-H16H	0.9800
C16C-H16I	0.9800
C17C-H17G	0.9800
C17C-H17H	0.9800
C17C-H17I	0.9800
C19C-C20C	1.459(9)
C20C-H20G	0.9800
C20C-H20H	0.9800
C20C-H20I	0.9800

Table 3. Bond lengths [Å] for ***cis*-5d**.

Molecule *cis*-**5d (d)**	
Pt1D-N3D	1.962(5)
Pt1D-N1D	1.994(5)
Pt1D-C18D	2.057(6)
Pt1D-N2D	2.119(5)
N1D-C1D	1.332(8)
N1D-C4D	1.378(8)
N2D-C5D	1.307(8)
N2D-C6D	1.438(8)
N3D-C19D	1.139(8)
C1D-C2D	1.379(9)
C1D-H1D	0.9500
C2D-C3D	1.380(9)
C2D-H2D	0.9500
C3D-C4D	1.369(9)
C3D-H3D	0.9500
C4D-C5D	1.415(9)
C5D-H5D	0.9500
C6D-C11D	1.387(8)
C6D-C7D	1.402(8)
C7D-C8D	1.391(9)
C7D-C12D	1.509(8)
C8D-C9D	1.367(9)
C8D-H8D	0.9500
C9D-C10D	1.366(10)
C9D-H9D	0.9500
C10D-C11D	1.415(9)
C10D-H10D	0.9500
C11D-C15D	1.491(9)
C12D-C13D	1.513(9)
C12D-C14D	1.520(8)
C12D-H12D	1.0000
C13D-H13J	0.9800
C13D-H13K	0.9800
C13D-H13L	0.9800
C14D-H14J	0.9800
C14D-H14K	0.9800
C14D-H14L	0.9800
C15D-C16D	1.513(8)
C15D-C17D	1.520(9)
C15D-H15D	1.0000
C16D-H16J	0.9800
C16D-H16K	0.9800
C16D-H16L	0.9800
C17D-H17J	0.9800
C17D-H17K	0.9800
C17D-H17L	0.9800
C19D-C20D	1.452(9)
C20D-H20J	0.9800
C20D-H20K	0.9800
C20D-H20L	0.9800

Table 3. Bond lengths [Å] for ***cis*-5d**.

Molecule *cis*-**5d (e)**	
Pt1E-N1E	1.977(5)
Pt1E-N3E	1.980(5)
Pt1E-C18E	2.063(6)
Pt1E-N2E	2.113(5)
N1E-C1E	1.338(7)
N1E-C4E	1.390(8)
N2E-C5E	1.309(8)
N2E-C6E	1.441(7)
N3E-C19E	1.123(7)
C1E-C2E	1.420(9)
C1E-H1E	0.9500
C2E-C3E	1.382(9)
C2E-H2E	0.9500
C3E-C4E	1.395(9)
C3E-H3E	0.9500
C4E-C5E	1.412(9)
C5E-H5E	0.9500
C6E-C7E	1.397(8)
C6E-C11E	1.413(8)
C7E-C8E	1.388(9)
C7E-C12E	1.523(8)
C8E-C9E	1.381(9)
C8E-H8E	0.9500
C9E-C10E	1.382(8)
C9E-H9E	0.9500
C10E-C11E	1.387(9)
C10E-H10E	0.9500
C11E-C15E	1.547(8)
C12E-C14E	1.470(11)
C12E-C13E	1.481(9)
C12E-H12E	1.0000
C13E-H13M	0.9800
C13E-H13N	0.9800
C13E-H13O	0.9800
C14E-H14M	0.9800
C14E-H14N	0.9800
C14E-H14O	0.9800
C15E-C17E	1.503(9)
C15E-C16E	1.517(9)
C15E-H15E	1.0000
C16E-H16M	0.9800
C16E-H16N	0.9800
C16E-H16O	0.9800
C17E-H17M	0.9800
C17E-H17N	0.9800
C17E-H17O	0.9800
C19E-C20E	1.468(9)
C20E-H20M	0.9800
C20E-H20N	0.9800
C20E-H20O	0.9800

Table 3. Bond lengths [Å] for ***cis*-5d**.

Molecule *cis*-**5d (f)**		C9F-H9F	0.9500
		C10F-C11F	1.385(9)
Pt1F-N3F	1.954(6)	C10F-H10F	0.9500
Pt1F-N1F	1.990(5)	C11F-C15F	1.540(8)
Pt1F-C18F	2.054(6)	C12F-C13F	1.520(8)
Pt1F-N2F	2.116(5)	C12F-C14F	1.527(9)
N1F-C1F	1.342(7)	C12F-H12F	1.0000
N1F-C4F	1.386(8)	C13F-H13P	0.9800
N2F-C5F	1.308(8)	C13F-H13Q	0.9800
N2F-C6F	1.439(8)	C13F-H13R	0.9800
N3F-C19F	1.136(8)	C14F-H14P	0.9800
C1F-C2F	1.408(9)	C14F-H14Q	0.9800
C1F-H1F	0.9500	C14F-H14R	0.9800
C2F-C3F	1.384(9)	C15F-C17F	1.495(9)
C2F-H2F	0.9500	C15F-C16F	1.534(9)
C3F-C4F	1.397(8)	C15F-H15F	1.0000
C3F-H3F	0.9500	C16F-H16P	0.9800
C4F-C5F	1.416(8)	C16F-H16Q	0.9800
C5F-H5F	0.9500	C16F-H16R	0.9800
C6F-C11F	1.411(8)	C17F-H17P	0.9800
C6F-C7F	1.418(8)	C17F-H17Q	0.9800
C7F-C8F	1.383(9)	C17F-H17R	0.9800
C7F-C12F	1.531(8)	C19F-C20F	1.451(9)
C8F-C9F	1.383(9)	C20F-H20P	0.9800
C8F-H8F	0.9500	C20F-H20Q	0.9800
C9F-C10F	1.396(8)	C20F-H20R	0.9800

Table 4. Bond angles [°] for ***cis*-5d**.

Molecule *cis*-**5d (a)**

N3A-Pt1A-N1A	172.6(2)
N3A-Pt1A-C18A	92.4(2)
N1A-Pt1A-C18A	94.5(2)
N3A-Pt1A-N2A	93.9(2)
N1A-Pt1A-N2A	79.2(2)
C18A-Pt1A-N2A	173.7(2)
C1A-N1A-C4A	107.5(5)
C1A-N1A-Pt1A	137.5(4)
C4A-N1A-Pt1A	114.6(4)
C5A-N2A-C6A	121.7(5)
C5A-N2A-Pt1A	112.1(4)
C6A-N2A-Pt1A	126.0(4)
C19A-N3A-Pt1A	172.8(6)
N1A-C1A-C2A	108.8(6)
N1A-C1A-H1A	125.6
C2A-C1A-H1A	125.6
C3A-C2A-C1A	107.9(6)
C3A-C2A-H2A	126.1
C1A-C2A-H2A	126.1
C2A-C3A-C4A	106.9(6)
C2A-C3A-H3A	126.6
C4A-C3A-H3A	126.6
N1A-C4A-C3A	108.9(6)
N1A-C4A-C5A	115.6(5)
C3A-C4A-C5A	135.4(6)
N2A-C5A-C4A	118.3(6)
N2A-C5A-H5A	120.9
C4A-C5A-H5A	120.9
C7A-C6A-C11A	123.1(6)
C7A-C6A-N2A	118.4(5)
C11A-C6A-N2A	118.5(5)
C8A-C7A-C6A	116.8(6)
C8A-C7A-C12A	121.3(6)
C6A-C7A-C12A	121.8(6)
C9A-C8A-C7A	121.5(7)
C9A-C8A-H8A	119.2
C7A-C8A-H8A	119.2
C8A-C9A-C10A	120.6(7)
C8A-C9A-H9A	119.7
C10A-C9A-H9A	119.7
C11A-C10A-C9A	120.9(7)
C11A-C10A-H10A	119.6
C9A-C10A-H10A	119.6
C10A-C11A-C6A	117.0(6)
C10A-C11A-C15A	121.2(6)
C6A-C11A-C15A	121.8(6)
C7A-C12A-C14A	113.0(6)
C7A-C12A-C13A	110.5(5)
C14A-C12A-C13A	109.2(5)
C7A-C12A-H12A	108.0
C14A-C12A-H12A	108.0
C13A-C12A-H12A	108.0
C12A-C13A-H13A	109.5
C12A-C13A-H13B	109.5
H13A-C13A-H13B	109.5
C12A-C13A-H13C	109.5
H13A-C13A-H13C	109.5
H13B-C13A-H13C	109.5
C12A-C14A-H14A	109.5
C12A-C14A-H14B	109.5
H14A-C14A-H14B	109.5
C12A-C14A-H14C	109.5
H14A-C14A-H14C	109.5
H14B-C14A-H14C	109.5
C11A-C15A-C16A	111.7(5)
C11A-C15A-C17A	112.7(6)
C16A-C15A-C17A	109.3(6)
C11A-C15A-H15A	107.6
C16A-C15A-H15A	107.6
C17A-C15A-H15A	107.6
C15A-C16A-H16A	109.5
C15A-C16A-H16B	109.5
H16A-C16A-H16B	109.5
C15A-C16A-H16C	109.5
H16A-C16A-H16C	109.5
H16B-C16A-H16C	109.5
C15A-C17A-H17A	109.5
C15A-C17A-H17B	109.5
H17A-C17A-H17B	109.5
C15A-C17A-H17C	109.5
H17A-C17A-H17C	109.5
H17B-C17A-H17C	109.5
N3A-C19A-C20A	178.8(7)
C19A-C20A-H20A	109.5
C19A-C20A-H20B	109.5
H20A-C20A-H20B	109.5
C19A-C20A-H20C	109.5
H20A-C20A-H20C	109.5
H20B-C20A-H20C	109.5

Table 4. Bond angles [°] for ***cis*-5d**.

Molecule *cis*-**5d (b)**

N3B-Pt1B-N1B	172.3(2)
N3B-Pt1B-C18B	92.0(3)
N1B-Pt1B-C18B	95.6(3)
N3B-Pt1B-N2b	92.8(2)
N1B-Pt1B-N2b	79.5(2)
C18B-Pt1B-N2b	175.0(3)
C1B-N1B-C4B	106.3(5)
C1B-N1B-Pt1B	138.9(5)
C4B-N1B-Pt1B	114.8(4)
C5B-N2b-C6B	123.3(5)
C5B-N2b-Pt1B	112.0(4)
C6B-N2b-Pt1B	124.6(4)
C19B-N3B-Pt1B	167.0(5)
N1B-C1B-C2b	110.7(6)
N1B-C1B-H1B	124.7
C2b-C1B-H1B	124.7
C3B-C2b-C1B	107.1(6)
C3B-C2b-H2b	126.5
C1B-C2b-H2b	126.5
C2b-C3B-C4B	106.9(6)
C2b-C3B-H3B	126.5
C4B-C3B-H3B	126.5
C3B-C4B-N1B	109.0(6)
C3B-C4B-C5B	136.0(7)
N1B-C4B-C5B	115.0(5)
N2b-C5B-C4B	118.6(6)
N2b-C5B-H5B	120.7
C4B-C5B-H5B	120.7
C11B-C6B-C7B	122.0(6)
C11B-C6B-N2b	118.7(6)
C7B-C6B-N2b	118.9(6)
C8B-C7B-C6B	118.1(6)
C8B-C7B-C12b	121.8(6)
C6B-C7B-C12b	120.1(6)
C7B-C8B-C9B	120.2(6)
C7B-C8B-H8B	119.9
C9B-C8B-H8B	119.9
C10B-C9B-C8B	121.1(7)
C10B-C9B-H9B	119.5
C8B-C9B-H9B	119.5
C9B-C10B-C11B	120.6(7)
C9B-C10B-H10B	119.7
C11B-C10B-H10B	119.7
C6B-C11B-C10B	117.9(6)
C6B-C11B-C15B	122.0(6)
C10B-C11B-C15B	120.0(6)
C14B-C12b-C7B	112.8(5)
C14B-C12b-C13B	110.4(5)
C7B-C12b-C13B	111.7(5)
C14B-C12b-H12b	107.2
C7B-C12b-H12b	107.2
C13B-C12b-H12b	107.2
C12b-C13B-H13D	109.5
C12b-C13B-H13E	109.5
H13D-C13B-H13E	109.5
C12b-C13B-H13F	109.5
H13D-C13B-H13F	109.5
H13E-C13B-H13F	109.5
C12b-C14B-H14D	109.5
C12b-C14B-H14E	109.5
H14D-C14B-H14E	109.5
C12b-C14B-H14F	109.5
H14D-C14B-H14F	109.5
H14E-C14B-H14F	109.5
C17B-C15B-C16B	110.2(6)
C17B-C15B-C11B	110.4(6)
C16B-C15B-C11B	112.3(6)
C17B-C15B-H15B	107.9
C16B-C15B-H15B	107.9
C11B-C15B-H15B	107.9
C15B-C16B-H16D	109.5
C15B-C16B-H16E	109.5
H16D-C16B-H16E	109.5
C15B-C16B-H16F	109.5
H16D-C16B-H16F	109.5
H16E-C16B-H16F	109.5
C15B-C17B-H17D	109.5
C15B-C17B-H17E	109.5
H17D-C17B-H17E	109.5
C15B-C17B-H17F	109.5
H17D-C17B-H17F	109.5
H17E-C17B-H17F	109.5
N3B-C19B-C20B	176.9(7)
C19B-C20B-H20D	109.5
C19B-C20B-H20E	109.5
H20D-C20B-H20E	109.5
C19B-C20B-H20F	109.5
H20D-C20B-H20F	109.5
H20E-C20B-H20F	109.5

Table 4. Bond angles [°] for ***cis*-5d**.

Molecule ***cis*-5d (c)**

N3C-Pt1C-N1C	171.9(2)
N3C-Pt1C-C18C	93.0(3)
N1C-Pt1C-C18C	95.0(2)
N3C-Pt1C-N2C	92.4(2)
N1C-Pt1C-N2C	79.6(2)
C18C-Pt1C-N2C	174.3(2)
C1C-N1C-C4C	108.0(5)
C1C-N1C-Pt1C	138.2(5)
C4C-N1C-Pt1C	113.9(4)
C5C-N2C-C6C	122.2(5)
C5C-N2C-Pt1C	113.0(4)
C6C-N2C-Pt1C	124.8(4)
C19C-N3C-Pt1C	167.5(5)
N1C-C1C-C2C	110.2(6)
N1C-C1C-H1C	124.9
C2C-C1C-H1C	124.9
C3C-C2C-C1C	106.6(5)
C3C-C2C-H2C	126.7
C1C-C2C-H2C	126.7
C4C-C3C-C2C	107.4(6)
C4C-C3C-H3C	126.3
C2C-C3C-H3C	126.3
C3C-C4C-N1C	107.8(6)
C3C-C4C-C5C	136.3(6)
N1C-C4C-C5C	115.8(5)
N2C-C5C-C4C	117.7(6)
N2C-C5C-H5C	121.1
C4C-C5C-H5C	121.1
C7C-C6C-C11C	122.9(6)
C7C-C6C-N2C	118.7(6)
C11C-C6C-N2C	117.9(6)
C8C-C7C-C6C	118.0(6)
C8C-C7C-C12C	121.3(6)
C6C-C7C-C12C	120.7(6)
C7C-C8C-C9C	120.5(6)
C7C-C8C-H8C	119.8
C9C-C8C-H8C	119.8
C10C-C9C-C8C	120.4(6)
C10C-C9C-H9C	119.8
C8C-C9C-H9C	119.8
C9C-C10C-C11C	121.2(6)
C9C-C10C-H10C	119.4
C11C-C10C-H10C	119.4
C10C-C11C-C6C	116.8(6)
C10C-C11C-C15C	122.3(6)
C6C-C11C-C15C	120.9(6)
C14C-C12C-C7C	113.2(5)
C14C-C12C-C13C	110.1(5)
C7C-C12C-C13C	111.6(5)
C14C-C12C-H12C	107.2
C7C-C12C-H12C	107.2
C13C-C12C-H12C	107.2
C12C-C13C-H13G	109.5
C12C-C13C-H13H	109.5
H13G-C13C-H13H	109.5
C12C-C13C-H13I	109.5
H13G-C13C-H13I	109.5
H13H-C13C-H13I	109.5
C12C-C14C-H14G	109.5
C12C-C14C-H14H	109.5
H14G-C14C-H14H	109.5
C12C-C14C-H14I	109.5
H14G-C14C-H14I	109.5
H14H-C14C-H14I	109.5
C11C-C15C-C16C	111.8(5)
C11C-C15C-C17C	112.3(5)
C16C-C15C-C17C	109.5(5)
C11C-C15C-H15C	107.7
C16C-C15C-H15C	107.7
C17C-C15C-H15C	107.7
C15C-C16C-H16G	109.5
C15C-C16C-H16H	109.5
H16G-C16C-H16H	109.5
C15C-C16C-H16I	109.5
H16G-C16C-H16I	109.5
H16H-C16C-H16I	109.5
C15C-C17C-H17G	109.5
C15C-C17C-H17H	109.5
H17G-C17C-H17H	109.5
C15C-C17C-H17I	109.5
H17G-C17C-H17I	109.5
H17H-C17C-H17I	109.5
N3C-C19C-C20C	177.1(7)
C19C-C20C-H20G	109.5
C19C-C20C-H20H	109.5
H20G-C20C-H20H	109.5
C19C-C20C-H20I	109.5
H20G-C20C-H20I	109.5
H20H-C20C-H20I	109.5

Table 4. Bond angles [°] for ***cis*-5d**.

Molecule *cis*-**5d (d)**

N3D-Pt1D-N1D	174.5(2)
N3D-Pt1D-C18D	90.6(2)
N1D-Pt1D-C18D	94.7(2)
N3D-Pt1D-N2D	95.3(2)
N1D-Pt1D-N2D	79.3(2)
C18D-Pt1D-N2D	173.9(2)
C1D-N1D-C4D	106.8(5)
C1D-N1D-Pt1D	138.0(5)
C4D-N1D-Pt1D	115.0(4)
C5D-N2D-C6D	121.0(5)
C5D-N2D-Pt1D	111.9(4)
C6D-N2D-Pt1D	126.5(4)
C19D-N3D-Pt1D	175.2(5)
N1D-C1D-C2D	110.8(6)
N1D-C1D-H1D	124.6
C2D-C1D-H1D	124.6
C1D-C2D-C3D	105.9(6)
C1D-C2D-H2D	127.1
C3D-C2D-H2D	127.1
C4D-C3D-C2D	107.8(7)
C4D-C3D-H3D	126.1
C2D-C3D-H3D	126.1
C3D-C4D-N1D	108.7(6)
C3D-C4D-C5D	135.9(7)
N1D-C4D-C5D	115.3(6)
N2D-C5D-C4D	118.4(6)
N2D-C5D-H5D	120.8
C4D-C5D-H5D	120.8
C11D-C6D-C7D	122.9(6)
C11D-C6D-N2D	119.2(6)
C7D-C6D-N2D	117.7(6)
C8D-C7D-C6D	116.5(6)
C8D-C7D-C12D	119.6(6)
C6D-C7D-C12D	123.8(6)
C9D-C8D-C7D	122.4(7)
C9D-C8D-H8D	118.8
C7D-C8D-H8D	118.8
C10D-C9D-C8D	120.0(7)
C10D-C9D-H9D	120.0
C8D-C9D-H9D	120.0
C9D-C10D-C11D	121.0(7)
C9D-C10D-H10D	119.5
C11D-C10D-H10D	119.5
C6D-C11D-C10D	117.1(6)
C6D-C11D-C15D	121.8(6)
C10D-C11D-C15D	121.0(6)
C7D-C12D-C13D	111.7(5)
C7D-C12D-C14D	111.9(5)
C13D-C12D-C14D	111.1(6)
C7D-C12D-H12D	107.3
C13D-C12D-H12D	107.3
C14D-C12D-H12D	107.3
C12D-C13D-H13J	109.5
C12D-C13D-H13K	109.5
H13J-C13D-H13K	109.5
C12D-C13D-H13L	109.5
H13J-C13D-H13L	109.5
H13K-C13D-H13L	109.5
C12D-C14D-H14J	109.5
C12D-C14D-H14K	109.5
H14J-C14D-H14K	109.5
C12D-C14D-H14L	109.5
H14J-C14D-H14L	109.5
H14K-C14D-H14L	109.5
C11D-C15D-C16D	111.5(6)
C11D-C15D-C17D	115.2(6)
C16D-C15D-C17D	108.8(5)
C11D-C15D-H15D	107.0
C16D-C15D-H15D	107.0
C17D-C15D-H15D	107.0
C15D-C16D-H16J	109.5
C15D-C16D-H16K	109.5
H16J-C16D-H16K	109.5
C15D-C16D-H16L	109.5
H16J-C16D-H16L	109.5
H16K-C16D-H16L	109.5
C15D-C17D-H17J	109.5
C15D-C17D-H17K	109.5
H17J-C17D-H17K	109.5
C15D-C17D-H17L	109.5
H17J-C17D-H17L	109.5
H17K-C17D-H17L	109.5
N3D-C19D-C20D	178.4(7)
C19D-C20D-H20J	109.5
C19D-C20D-H20K	109.5
H20J-C20D-H20K	109.5
C19D-C20D-H20L	109.5
H20J-C20D-H20L	109.5
H20K-C20D-H20L	109.5

Table 4. Bond angles [°] for ***cis*-5d**.

Molecule ***cis*-5d (e)**

N1E-Pt1E-N3E	171.67(19)
N1E-Pt1E-C18E	94.4(2)
N3E-Pt1E-C18E	93.3(2)
N1E-Pt1E-N2E	79.6(2)
N3E-Pt1E-N2E	92.9(2)
C18E-Pt1E-N2E	173.3(2)
C1E-N1E-C4E	107.2(5)
C1E-N1E-Pt1E	138.1(5)
C4E-N1E-Pt1E	114.6(4)
C5E-N2E-C6E	120.7(5)
C5E-N2E-Pt1E	112.6(4)
C6E-N2E-Pt1E	126.7(4)
C19E-N3E-Pt1E	166.7(5)
N1E-C1E-C2E	109.9(6)
N1E-C1E-H1E	125.0
C2E-C1E-H1E	125.0
C3E-C2E-C1E	106.6(6)
C3E-C2E-H2E	126.7
C1E-C2E-H2E	126.7
C2E-C3E-C4E	107.0(6)
C2E-C3E-H3E	126.5
C4E-C3E-H3E	126.5
N1E-C4E-C3E	109.2(6)
N1E-C4E-C5E	116.0(6)
C3E-C4E-C5E	134.8(6)
N2E-C5E-C4E	117.2(6)
N2E-C5E-H5E	121.4
C4E-C5E-H5E	121.4
C7E-C6E-C11E	122.3(6)
C7E-C6E-N2E	119.0(5)
C11E-C6E-N2E	118.3(5)
C8E-C7E-C6E	116.8(6)
C8E-C7E-C12E	121.7(6)
C6E-C7E-C12E	121.4(6)
C9E-C8E-C7E	122.2(6)
C9E-C8E-H8E	118.9
C7E-C8E-H8E	118.9
C8E-C9E-C10E	120.0(6)
C8E-C9E-H9E	120.0
C10E-C9E-H9E	120.0
C9E-C10E-C11E	120.6(6)
C9E-C10E-H10E	119.7
C11E-C10E-H10E	119.7
C10E-C11E-C6E	118.0(6)
C10E-C11E-C15E	121.5(6)
C6E-C11E-C15E	120.5(6)
C14E-C12E-C13E	113.1(6)
C14E-C12E-C7E	110.5(6)
C13E-C12E-C7E	113.1(6)
C14E-C12E-H12E	106.5
C13E-C12E-H12E	106.5
C7E-C12E-H12E	106.5
C12E-C13E-H13M	109.5
C12E-C13E-H13N	109.5
H13M-C13E-H13N	109.5
C12E-C13E-H13O	109.5
H13M-C13E-H13O	109.5
H13N-C13E-H13O	109.5
C12E-C14E-H14M	109.5
C12E-C14E-H14N	109.5
H14M-C14E-H14N	109.5
C12E-C14E-H14O	109.5
H14M-C14E-H14O	109.5
H14N-C14E-H14O	109.5
C17E-C15E-C16E	109.8(6)
C17E-C15E-C11E	113.5(5)
C16E-C15E-C11E	110.4(5)
C17E-C15E-H15E	107.6
C16E-C15E-H15E	107.6
C11E-C15E-H15E	107.6
C15E-C16E-H16M	109.5
C15E-C16E-H16N	109.5
H16M-C16E-H16N	109.5
C15E-C16E-H16O	109.5
H16M-C16E-H16O	109.5
H16N-C16E-H16O	109.5
C15E-C17E-H17M	109.5
C15E-C17E-H17N	109.5
H17M-C17E-H17N	109.5
C15E-C17E-H17O	109.5
H17M-C17E-H17O	109.5
H17N-C17E-H17O	109.5
N3E-C19E-C20E	178.1(7)
C19E-C20E-H20M	109.5
C19E-C20E-H20N	109.5
H20M-C20E-H20N	109.5
C19E-C20E-H20O	109.5
H20M-C20E-H20O	109.5
H20N-C20E-H20O	109.5

Table 4. Bond angles [°] for ***cis*-5d**.

Molecule *cis*-**5d (f)**

N3F-Pt1F-N1F	171.60(19)	C10F-C11F-C15F	121.7(6)
N3F-Pt1F-C18F	91.5(2)	C6F-C11F-C15F	120.2(6)
N1F-Pt1F-C18F	96.2(2)	C13F-C12F-C14F	110.7(5)
N3F-Pt1F-N2F	92.9(2)	C13F-C12F-C7F	112.5(5)
N1F-Pt1F-N2F	79.4(2)	C14F-C12F-C7F	110.3(5)
C18F-Pt1F-N2F	175.5(2)	C13F-C12F-H12F	107.7
C1F-N1F-C4F	108.1(5)	C14F-C12F-H12F	107.7
C1F-N1F-Pt1F	137.2(5)	C7F-C12F-H12F	107.7
C4F-N1F-Pt1F	114.4(4)	C12F-C13F-H13P	109.5
C5F-N2F-C6F	121.6(5)	C12F-C13F-H13Q	109.5
C5F-N2F-Pt1F	112.7(4)	H13P-C13F-H13Q	109.5
C6F-N2F-Pt1F	125.5(4)	C12F-C13F-H13R	109.5
C19F-N3F-Pt1F	167.0(5)	H13P-C13F-H13R	109.5
N1F-C1F-C2F	108.8(6)	H13Q-C13F-H13R	109.5
N1F-C1F-H1F	125.6	C12F-C14F-H14P	109.5
C2F-C1F-H1F	125.6	C12F-C14F-H14Q	109.5
C3F-C2F-C1F	107.8(6)	H14P-C14F-H14Q	109.5
C3F-C2F-H2F	126.1	C12F-C14F-H14R	109.5
C1F-C2F-H2F	126.1	H14P-C14F-H14R	109.5
C2F-C3F-C4F	106.4(6)	H14Q-C14F-H14R	109.5
C2F-C3F-H3F	126.8	C17F-C15F-C16F	110.4(6)
C4F-C3F-H3F	126.8	C17F-C15F-C11F	113.2(6)
N1F-C4F-C3F	108.9(6)	C16F-C15F-C11F	110.9(5)
N1F-C4F-C5F	116.1(6)	C17F-C15F-H15F	107.4
C3F-C4F-C5F	134.9(6)	C16F-C15F-H15F	107.4
N2F-C5F-C4F	117.2(6)	C11F-C15F-H15F	107.4
N2F-C5F-H5F	121.4	C15F-C16F-H16P	109.5
C4F-C5F-H5F	121.4	C15F-C16F-H16Q	109.5
C11F-C6F-C7F	121.2(6)	H16P-C16F-H16Q	109.5
C11F-C6F-N2F	119.1(5)	C15F-C16F-H16R	109.5
C7F-C6F-N2F	119.4(5)	H16P-C16F-H16R	109.5
C8F-C7F-C6F	117.9(6)	H16Q-C16F-H16R	109.5
C8F-C7F-C12F	121.6(6)	C15F-C17F-H17P	109.5
C6F-C7F-C12F	120.5(6)	C15F-C17F-H17Q	109.5
C7F-C8F-C9F	122.2(6)	H17P-C17F-H17Q	109.5
C7F-C8F-H8F	118.9	C15F-C17F-H17R	109.5
C9F-C8F-H8F	118.9	H17P-C17F-H17R	109.5
C8F-C9F-C10F	119.0(6)	H17Q-C17F-H17R	109.5
C8F-C9F-H9F	120.5	N3F-C19F-C20F	175.0(7)
C10F-C9F-H9F	120.5	C19F-C20F-H20P	109.5
C11F-C10F-C9F	121.7(6)	C19F-C20F-H20Q	109.5
C11F-C10F-H10F	119.1	H20P-C20F-H20Q	109.5
C9F-C10F-H10F	119.1	C19F-C20F-H20R	109.5
C10F-C11F-C6F	118.1(5)	H20P-C20F-H20R	109.5
		H20Q-C20F-H20R	109.5

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for ***cis*-5d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

Molecule ***cis*-5d (a)**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt1A	134(1)	108(1)	130(1)	-2(1)	7(1)	1(1)
N1A	150(30)	160(30)	70(30)	-30(20)	-10(20)	-20(20)
N2A	150(30)	120(30)	120(30)	-40(20)	-30(20)	0(20)
N3A	210(30)	170(30)	150(30)	30(20)	10(20)	60(30)
C1A	240(40)	180(40)	160(30)	20(30)	20(30)	0(30)
C2A	300(40)	210(40)	290(40)	-20(30)	80(30)	-130(30)
C3A	190(40)	310(40)	200(40)	-30(30)	-20(30)	-100(30)
C4A	230(40)	140(30)	110(30)	-30(30)	40(30)	-30(30)
C5A	160(40)	190(40)	260(40)	-10(30)	40(30)	0(30)
C6A	90(30)	160(40)	180(30)	-40(30)	-10(30)	10(30)
C7A	150(30)	170(40)	230(40)	30(30)	40(30)	50(30)
C8A	360(50)	290(40)	230(40)	20(30)	0(30)	-20(30)
C9A	470(50)	140(40)	430(50)	-10(40)	-50(40)	30(40)
C10A	330(40)	200(40)	350(50)	-110(30)	-70(40)	70(30)
C11A	140(30)	200(40)	160(30)	-40(30)	-20(30)	10(30)
C12A	150(30)	170(40)	260(40)	0(30)	10(30)	20(30)
C13A	330(40)	490(50)	270(40)	-100(40)	10(30)	-60(40)
C14A	440(50)	320(50)	200(40)	70(30)	140(30)	30(40)
C15A	250(40)	210(40)	190(40)	-30(30)	-20(30)	60(30)
C16A	260(40)	410(50)	380(50)	-70(40)	-10(40)	-100(40)
C17A	260(40)	340(50)	320(40)	-90(40)	-20(30)	-30(30)
C18A	120(30)	230(40)	180(40)	-10(30)	60(30)	80(30)
C19A	120(30)	200(40)	160(30)	0(30)	50(30)	50(30)
C20A	220(40)	290(40)	290(40)	80(30)	-50(30)	-150(30)

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for ***cis*-5d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

Molecule *cis*-**5d (b)**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt1B	168(1)	162(1)	164(1)	23(1)	29(1)	6(1)
N1B	150(30)	170(30)	190(30)	40(20)	0(20)	70(20)
N2b	210(30)	150(30)	140(30)	-20(20)	80(20)	-30(20)
N3B	140(30)	220(30)	190(30)	-30(30)	10(20)	-40(20)
C1B	240(40)	270(40)	210(40)	40(30)	90(30)	30(30)
C2b	250(40)	330(40)	150(40)	30(30)	50(30)	150(30)
C3B	170(40)	270(40)	210(40)	-60(30)	-30(30)	70(30)
C4B	190(40)	200(40)	160(30)	-10(30)	70(30)	90(30)
C5B	180(40)	170(40)	170(30)	-40(30)	40(30)	40(30)
C6B	120(30)	100(30)	220(40)	10(30)	10(30)	-40(30)
C7B	100(30)	180(40)	210(30)	0(30)	-10(30)	-60(30)
C8B	240(40)	200(40)	310(40)	30(30)	30(30)	20(30)
C9B	370(50)	300(50)	160(40)	80(30)	20(30)	-50(30)
C10B	280(40)	180(40)	280(40)	-60(30)	40(30)	-40(30)
C11B	210(40)	160(40)	200(40)	10(30)	80(30)	-20(30)
C12b	160(30)	190(40)	200(40)	30(30)	30(30)	20(30)
C13B	240(40)	210(40)	230(40)	-20(30)	10(30)	40(30)
C14B	240(40)	430(50)	180(40)	10(30)	40(30)	100(30)
C15B	460(50)	180(40)	170(40)	20(30)	130(30)	90(30)
C16B	320(40)	240(40)	470(50)	-40(40)	30(40)	40(30)
C17B	410(50)	220(50)	620(60)	-140(40)	160(40)	20(40)
C18B	260(40)	330(50)	450(50)	50(40)	120(40)	-140(30)
C19B	240(40)	170(40)	230(40)	-100(30)	30(30)	-110(30)
C20B	300(40)	320(50)	260(40)	10(30)	-80(30)	-60(30)

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for ***cis*-5d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

Molecule *cis*-**5d (c)**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt1C	157(1)	150(1)	126(1)	-2(1)	21(1)	11(1)
N1C	170(30)	210(30)	140(30)	-40(20)	40(20)	30(20)
N2C	160(30)	130(30)	140(30)	0(20)	40(20)	70(20)
N3C	190(30)	190(30)	180(30)	-20(30)	40(20)	10(20)
C1C	280(40)	150(40)	120(30)	0(30)	90(30)	20(30)
C2C	290(40)	300(40)	80(30)	30(30)	40(30)	140(30)
C3C	240(40)	210(40)	100(30)	-50(30)	-20(30)	70(30)
C4C	220(40)	160(40)	100(30)	-40(30)	10(30)	20(30)
C5C	100(30)	200(40)	220(40)	-30(30)	-30(30)	80(30)
C6C	150(30)	170(40)	140(30)	20(30)	-50(30)	-60(30)
C7C	140(30)	150(40)	210(40)	0(30)	-50(30)	-60(30)
C8C	200(40)	240(40)	120(30)	-20(30)	30(30)	-50(30)
C9C	250(40)	270(40)	170(40)	110(30)	-40(30)	-50(30)
C10C	170(40)	210(40)	200(40)	0(30)	0(30)	30(30)
C11C	170(40)	200(40)	150(30)	40(30)	-30(30)	-50(30)
C12C	140(30)	210(40)	230(40)	0(30)	90(30)	-10(30)
C13C	260(40)	260(40)	340(40)	10(30)	40(30)	100(30)
C14C	290(40)	240(40)	330(40)	-90(30)	60(30)	80(30)
C15C	170(40)	130(40)	290(40)	10(30)	30(30)	10(30)
C16C	310(40)	160(40)	270(40)	0(30)	20(30)	20(30)
C17C	270(40)	260(40)	340(40)	0(40)	10(30)	60(30)
C18C	200(40)	290(40)	370(40)	50(40)	140(30)	-140(30)
C19C	120(30)	170(40)	230(40)	-80(30)	50(30)	-50(30)
C20C	430(50)	230(40)	80(30)	-40(30)	20(30)	40(30)

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for ***cis*-5d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

Molecule *cis*-**5d (d)**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt1D	165(1)	123(1)	132(1)	13(1)	6(1)	-8(1)
N1D	260(30)	140(30)	90(30)	0(20)	-10(20)	-10(20)
N2D	110(30)	140(30)	200(30)	50(20)	-40(20)	40(20)
N3D	110(30)	160(30)	170(30)	30(20)	30(20)	40(20)
C1D	290(40)	130(40)	130(30)	20(30)	-30(30)	10(30)
C2D	340(40)	140(40)	370(50)	40(30)	-40(40)	-50(30)
C3D	250(40)	220(40)	350(40)	20(30)	-40(30)	-50(30)
C4D	190(40)	210(40)	230(40)	60(30)	-50(30)	-10(30)
C5D	130(30)	280(40)	190(40)	70(30)	-80(30)	-10(30)
C6D	140(30)	150(40)	180(30)	50(30)	-10(30)	-10(30)
C7D	140(30)	180(40)	180(30)	30(30)	-30(30)	10(30)
C8D	290(40)	210(40)	250(40)	-30(30)	10(30)	30(30)
C9D	510(50)	130(40)	470(50)	70(40)	-20(40)	60(40)
C10D	350(40)	210(40)	370(50)	180(40)	-20(40)	30(30)
C11D	160(30)	210(40)	150(30)	30(30)	0(30)	40(30)
C12D	260(40)	210(40)	110(30)	20(30)	60(30)	70(30)
C13D	310(50)	350(50)	520(50)	60(40)	170(40)	-30(40)
C14D	290(40)	300(50)	320(40)	70(40)	50(30)	-70(30)
C15D	280(40)	250(40)	150(30)	150(30)	-30(30)	-50(30)
C16D	310(50)	420(50)	420(50)	90(40)	20(40)	-110(40)
C17D	290(40)	480(50)	360(50)	190(40)	40(40)	-50(40)
C18D	270(40)	180(40)	150(30)	-10(30)	10(30)	120(30)
C19D	120(30)	250(40)	170(40)	30(30)	-70(30)	60(30)
C20D	180(40)	240(40)	240(40)	60(30)	-70(30)	-70(30)

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for ***cis*-5d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

Molecule *cis*-**5d (e)**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt1E	147(1)	142(1)	141(1)	-6(1)	4(1)	-14(1)
N1E	160(30)	110(30)	110(30)	10(20)	10(20)	20(20)
N2E	150(30)	140(30)	160(30)	-30(20)	10(20)	-20(20)
N3E	110(30)	150(30)	180(30)	20(20)	-30(20)	-40(20)
C1E	270(40)	200(40)	120(30)	-20(30)	-70(30)	50(30)
C2E	230(40)	240(40)	180(40)	-70(30)	-60(30)	100(30)
C3E	220(40)	260(40)	240(40)	80(30)	20(30)	90(30)
C4E	140(30)	150(40)	250(40)	10(30)	10(30)	50(30)
C5E	120(30)	140(40)	270(40)	30(30)	10(30)	0(30)
C6E	200(40)	90(30)	220(40)	-60(30)	50(30)	-60(30)
C7E	160(30)	80(30)	330(40)	-50(30)	-40(30)	0(30)
C8E	280(40)	250(40)	320(40)	-90(40)	-150(30)	0(30)
C9E	320(40)	240(40)	230(40)	-130(30)	-50(30)	60(30)
C10E	210(40)	160(40)	260(40)	0(30)	60(30)	40(30)
C11E	150(30)	180(40)	190(30)	10(30)	10(30)	-10(30)
C12E	290(40)	210(40)	330(40)	-100(30)	-160(30)	70(30)
C13E	260(40)	320(50)	650(60)	-180(40)	40(40)	120(40)
C14E	340(50)	400(60)	1230(90)	310(60)	0(60)	80(40)
C15E	260(40)	170(40)	190(30)	-70(30)	50(30)	60(30)
C16E	410(50)	410(50)	200(40)	20(40)	-10(40)	-100(40)
C17E	250(40)	460(50)	320(40)	-40(40)	-50(30)	60(40)
C18E	170(40)	180(40)	220(40)	10(30)	-60(30)	-140(30)
C19E	200(40)	170(40)	120(30)	40(30)	20(30)	-10(30)
C20E	300(40)	260(40)	210(40)	-10(30)	90(30)	0(30)

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for ***cis*-5d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

Molecule *cis*-**5d (f)**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt1F	146(1)	154(1)	142(1)	-10(1)	1(1)	-24(1)
N1F	130(30)	180(30)	130(30)	-80(20)	-20(20)	0(20)
N2F	100(30)	170(30)	240(30)	-10(20)	-20(20)	-40(20)
N3F	160(30)	210(30)	160(30)	-10(30)	-20(20)	-40(20)
C1F	210(40)	160(40)	170(30)	0(30)	-80(30)	30(30)
C2F	320(40)	270(40)	60(30)	-30(30)	-20(30)	50(30)
C3F	190(40)	250(40)	130(30)	30(30)	10(30)	60(30)
C4F	120(30)	170(40)	200(30)	40(30)	-60(30)	40(30)
C5F	100(30)	180(40)	170(30)	30(30)	0(30)	10(30)
C6F	180(30)	120(30)	150(30)	0(30)	30(30)	-90(30)
C7F	170(30)	120(40)	230(40)	10(30)	10(30)	-60(30)
C8F	240(40)	200(40)	200(40)	-10(30)	-70(30)	-30(30)
C9F	330(40)	180(40)	180(40)	-30(30)	-10(30)	-30(30)
C10F	190(40)	120(40)	290(40)	70(30)	70(30)	40(30)
C11F	140(30)	200(40)	170(30)	50(30)	30(30)	-30(30)
C12F	260(40)	170(40)	140(30)	10(30)	-60(30)	-20(30)
C13F	320(40)	200(40)	440(50)	-20(40)	-90(40)	20(30)
C14F	370(40)	180(40)	300(40)	40(30)	-50(30)	-10(30)
C15F	190(40)	170(40)	260(40)	0(30)	10(30)	20(30)
C16F	350(50)	390(50)	250(40)	80(40)	-110(40)	-40(40)
C17F	210(40)	400(50)	330(40)	-30(40)	-120(30)	40(30)
C18F	200(40)	170(40)	330(40)	-20(30)	-40(30)	-120(30)
C19F	180(40)	140(40)	240(40)	60(30)	-30(30)	-100(30)
C20F	300(40)	260(40)	240(40)	10(30)	40(30)	-50(30)

Table 6. Hydrogen coordinates (x 10^3) and isotropic displacement parameters (Å^{2}x 10^3) for ***cis*-5d**.

Molecule *cis*-**5d (a)**

	x	y	z	Uiso
H1A	42	904	117	23
H2A	142	952	108	32
H3A	197	772	114	28
H5A	159	533	127	24
H8A	68	184	184	35
H9A	74	71	140	41
H10A	81	155	91	35
H12A	56	491	185	23
H13A	144	353	211	43
H13B	126	477	225	43
H13C	153	467	191	43
H14A	-5	356	207	38
H14B	31	417	234	38
H14C	46	289	223	38
H15A	73	460	76	26
H16A	168	417	75	42
H16B	144	407	40	42
H16C	156	292	60	42
H17A	55	241	46	37
H17B	47	364	30	37
H17C	6	327	57	37
H20A	-97	260	113	32
H20B	-144	325	132	32
H20C	-95	259	150	32

Molecule *cis*-**5d (b)**

	x	y	z	U_{iso}
H1B	346	556	139	29
H2b	261	502	108	30
H3B	214	342	137	26
H5B	247	224	196	21
H8B	374	-34	269	30
H9B	328	23	313	33
H10B	279	196	314	30
H12b	393	140	202	22
H13D	325	-61	199	27
H13E	364	-22	171	27
H13F	313	59	181	27
H14D	452	24	237	34
H14E	457	-4	201	34
H14F	421	-87	223	34
H15B	259	389	249	33
H16D	200	313	302	41
H16E	181	286	267	41
H16F	182	416	279	41
H17D	269	512	293	50
H17E	327	457	283	50
H17F	295	406	312	50
H20D	464	336	311	35
H20E	495	241	290	35
H20F	433	218	301	35

Table 6. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for ***cis*-5d**.

Molecule *cis*-**5d (c)**

	x	y	z	U_{iso}
H1C	147	487	351	22
H2C	233	526	383	27
H3C	280	696	358	22
H5C	250	829	300	21
H8C	216	878	181	23
H9C	172	1058	186	28
H10C	131	1110	233	23
H12C	210	652	236	23
H13G	314	752	221	35
H13H	305	627	237	35
H13I	292	742	256	35
H14G	191	663	182	34
H14H	242	579	190	34
H14I	253	706	177	34
H15C	105	920	296	24
H16G	189	979	318	30
H16H	141	1061	331	30
H16I	181	1107	304	30
H17G	53	1089	302	35
H17H	49	1053	266	35
H17I	89	1156	277	35
H20G	72	838	189	30
H20H	11	849	203	30
H20I	28	736	184	30

Molecule *cis*-**5d (d)**

	x	y	z	U_{iso}
H1D	447	144	369	22
H2D	348	95	376	34
H3D	297	284	381	33
H5D	338	524	380	24
H8D	417	855	435	30
H9D	430	979	393	44
H10D	441	908	343	37
H12D	420	546	431	23
H13J	343	708	455	47
H13K	354	585	471	47
H13L	328	593	436	47
H14J	491	667	454	36
H14K	457	594	479	36
H14L	444	729	474	36
H15D	451	607	324	27
H16J	356	643	317	46
H16K	387	647	285	46
H16L	369	765	302	46
H17J	466	829	297	45
H17K	485	708	282	45
H17L	515	758	313	45
H20J	649	696	367	27
H20K	611	760	393	27
H20L	600	779	356	27

Table 6. Hydrogen coordinates (x 10^3) and isotropic displacement parameters (Å^{2}x 10^3) for ***cis*-5d**.

Molecule *cis*-**5d (e)**

	x	y	z	U_{iso}
H1E	347	594	598	24
H2E	263	553	631	26
H3E	220	370	610	29
H5E	257	214	559	21
H8E	263	96	449	34
H9E	330	-46	451	32
H10E	395	-46	492	25
H12E	232	302	508	33
H13M	160	302	472	50
H13N	172	173	484	50
H13O	193	212	451	50
H14M	271	359	448	79
H14N	298	401	480	79
H14O	237	442	471	79
H15E	412	175	550	25
H16M	376	-54	564	41
H16N	348	62	576	41
H16O	410	28	588	41
H17M	459	-35	528	41
H17N	487	49	553	41
H17O	479	92	518	41
H20M	469	199	453	31
H20N	468	323	436	31
H20O	413	247	436	31

Molecule *cis*-**5d (f)**

	x	y	z	U_{iso}
H1F	850	607	97	22
H2F	763	572	128	26
H3F	721	384	110	23
H5F	759	223	60	18
H8F	770	93	-49	26
H9F	839	-48	-45	27
H10F	902	-45	-3	24
H12F	735	299	8	22
H13P	707	223	-54	39
H13Q	668	301	-32	39
H13R	681	169	-23	39
H14P	805	409	-15	34
H14Q	746	446	-30	34
H14R	787	364	-49	34
H15F	917	179	53	25
H16P	875	-44	69	40
H16Q	850	77	81	40
H16R	911	37	93	40
H17P	962	-39	37	38
H17Q	991	58	58	38
H17R	981	80	21	38
H20P	990	233	-46	32
H20Q	946	311	-65	32
H20R	927	191	-50	32

Table 7. Principal mean square atomic displacements U

Molecule *cis*-**5d (a)**				Molecule *cis*-**5d (b)**			
0.0137	0.0126	0.0108	Pt1A	0.0202	0.0159	0.0132	Pt1B
0.0176	0.0146	0.0056	N1A	0.0239	0.0180	0.0083	N1B
0.0183	0.0134	0.0075	N2A	0.0261	0.0140	0.0092	N2b
0.0258	0.0152	0.0116	N3A	0.0247	0.0182	0.0125	N3B
0.0247	0.0192	0.0144	C1A	0.0340	0.0239	0.0137	C1B
0.0427	0.0257	0.0107	C2A	0.0455	0.0167	0.0119	C2b
0.0369	0.0211	0.0116	C3A	0.0341	0.0171	0.0135	C3B
0.0248	0.0131	0.0095	C4A	0.0303	0.0178	0.0073	C4B
0.0269	0.0188	0.0144	C5A	0.0216	0.0206	0.0092	C5B
0.0220	0.0126	0.0087	C6A	0.0222	0.0157	0.0067	C6B
0.0269	0.0169	0.0114	C7A	0.0220	0.0204	0.0069	C7B
0.0372	0.0282	0.0226	C8A	0.0325	0.0234	0.0189	C8B
0.0512	0.0385	0.0135	C9A	0.0395	0.0312	0.0123	C9B
0.0482	0.0263	0.0131	C10A	0.0342	0.0250	0.0149	C10B
0.0230	0.0156	0.0116	C11A	0.0284	0.0169	0.0116	C11B
0.0258	0.0181	0.0136	C12A	0.0237	0.0163	0.0143	C12b
0.0543	0.0309	0.0231	C13A	0.0267	0.0236	0.0172	C13B
0.0515	0.0314	0.0125	C14A	0.0476	0.0221	0.0153	C14B
0.0304	0.0185	0.0161	C15A	0.0536	0.0162	0.0120	C15B
0.0491	0.0368	0.0196	C16A	0.0479	0.0338	0.0217	C16B
0.0426	0.0287	0.0211	C17A	0.0722	0.0363	0.0157	C17B
0.0271	0.0202	0.0053	C18A	0.0501	0.0428	0.0109	C18B
0.0233	0.0167	0.0073	C19A	0.0368	0.0202	0.0064	C19B
0.0463	0.0241	0.0097	C20A	0.0399	0.0293	0.0184	C20B

Table 7. Principal mean square atomic displacements U

Molecule *cis*-**5d (c)**				Molecule *cis*-**5d (d)**			
0.0170	0.0147	0.0116	Pt1C	0.0166	0.0141	0.0112	Pt1D
0.0237	0.0187	0.0092	N1C	0.0261	0.0143	0.0088	N1D
0.0228	0.0136	0.0061	N2C	0.0226	0.0163	0.0060	N2D
0.0224	0.0197	0.0136	N3C	0.0220	0.0141	0.0089	N3D
0.0321	0.0149	0.0086	C1C	0.0301	0.0152	0.0108	C1D
0.0438	0.0160	0.0073	C2C	0.0419	0.0307	0.0129	C2D
0.0308	0.0154	0.0081	C3C	0.0381	0.0257	0.0185	C3D
0.0224	0.0171	0.0081	C4C	0.0308	0.0186	0.0142	C4D
0.0279	0.0187	0.0055	C5C	0.0332	0.0201	0.0067	C5D
0.0244	0.0128	0.0084	C6C	0.0218	0.0133	0.0119	C6D
0.0249	0.0176	0.0081	C7C	0.0208	0.0177	0.0112	C7D
0.0285	0.0172	0.0107	C8C	0.0304	0.0262	0.0183	C8D
0.0376	0.0215	0.0099	C9C	0.0525	0.0474	0.0104	C9D
0.0230	0.0200	0.0154	C10C	0.0484	0.0352	0.0088	C10D
0.0262	0.0141	0.0128	C11C	0.0237	0.0152	0.0121	C11D
0.0281	0.0206	0.0085	C12C	0.0329	0.0164	0.0091	C12D
0.0386	0.0322	0.0156	C13C	0.0610	0.0359	0.0198	C13D
0.0379	0.0350	0.0132	C14C	0.0379	0.0349	0.0174	C14D
0.0292	0.0165	0.0132	C15C	0.0387	0.0248	0.0039	C15D
0.0323	0.0266	0.0160	C16C	0.0537	0.0397	0.0217	C16D
0.0344	0.0318	0.0206	C17C	0.0624	0.0318	0.0192	C17D
0.0448	0.0365	0.0038	C18C	0.0352	0.0151	0.0096	C18D
0.0312	0.0120	0.0089	C19C	0.0272	0.0226	0.0051	C19D
0.0444	0.0235	0.0071	C20C	0.0358	0.0186	0.0125	C20D

Table 7. Principal mean square atomic displacements U

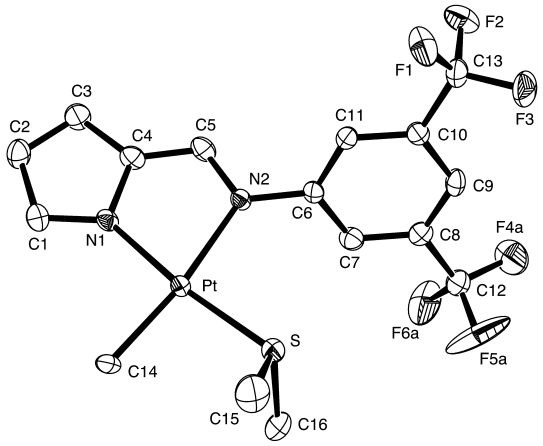
Molecule *cis*-**5d (e)**				Molecule *cis*-**5d (f)**			
0.0160	0.0141	0.0129	Pt1E	0.0176	0.0143	0.0122	Pt1F
0.0170	0.0108	0.0095	N1E	0.0243	0.0133	0.0069	N1F
0.0190	0.0145	0.0108	N2E	0.0246	0.0195	0.0079	N2F
0.0211	0.0144	0.0087	N3E	0.0233	0.0181	0.0125	N3F
0.0328	0.0170	0.0092	C1E	0.0277	0.0164	0.0102	C1F
0.0377	0.0137	0.0136	C2E	0.0355	0.0234	0.0052	C2F
0.0375	0.0208	0.0135	C3E	0.0299	0.0157	0.0121	C3F
0.0255	0.0191	0.0099	C4E	0.0238	0.0194	0.0065	C4F
0.0274	0.0139	0.0122	C5E	0.0210	0.0142	0.0103	C5F
0.0289	0.0165	0.0058	C6E	0.0247	0.0147	0.0051	C6F
0.0354	0.0146	0.0068	C7E	0.0235	0.0208	0.0073	C7F
0.0474	0.0257	0.0122	C8E	0.0302	0.0208	0.0129	C8F
0.0433	0.0255	0.0104	C9E	0.0335	0.0207	0.0144	C9F
0.0301	0.0202	0.0127	C10E	0.0349	0.0151	0.0094	C10F
0.0194	0.0180	0.0140	C11E	0.0242	0.0178	0.0097	C11F
0.0521	0.0172	0.0134	C12E	0.0286	0.0162	0.0113	C12F
0.0734	0.0373	0.0134	C13E	0.0498	0.0268	0.0201	C13F
0.1332	0.0403	0.0244	C14E	0.0400	0.0287	0.0166	C14F
0.0297	0.0248	0.0080	C15E	0.0259	0.0204	0.0160	C15F
0.0511	0.0312	0.0195	C16E	0.0492	0.0334	0.0167	C16F
0.0494	0.0318	0.0218	C17E	0.0454	0.0360	0.0137	C17F
0.0330	0.0206	0.0031	C18E	0.0351	0.0301	0.0055	C18F
0.0209	0.0191	0.0100	C19E	0.0320	0.0192	0.0049	C19F
0.0356	0.0263	0.0154	C20E	0.0334	0.0253	0.0206	C20F

References

(1)Farrugia, L. J. *J. Appl. Crys.* **1997**, *30*, 565.

2. $(SMe_2)Pt[iminopyrrolide(3,5\text{-}(CF_3)_2C_6H_3)]Me$ (*cis*-2c)

Contents



$C_{16}H_{16}F_6N_2PtS$

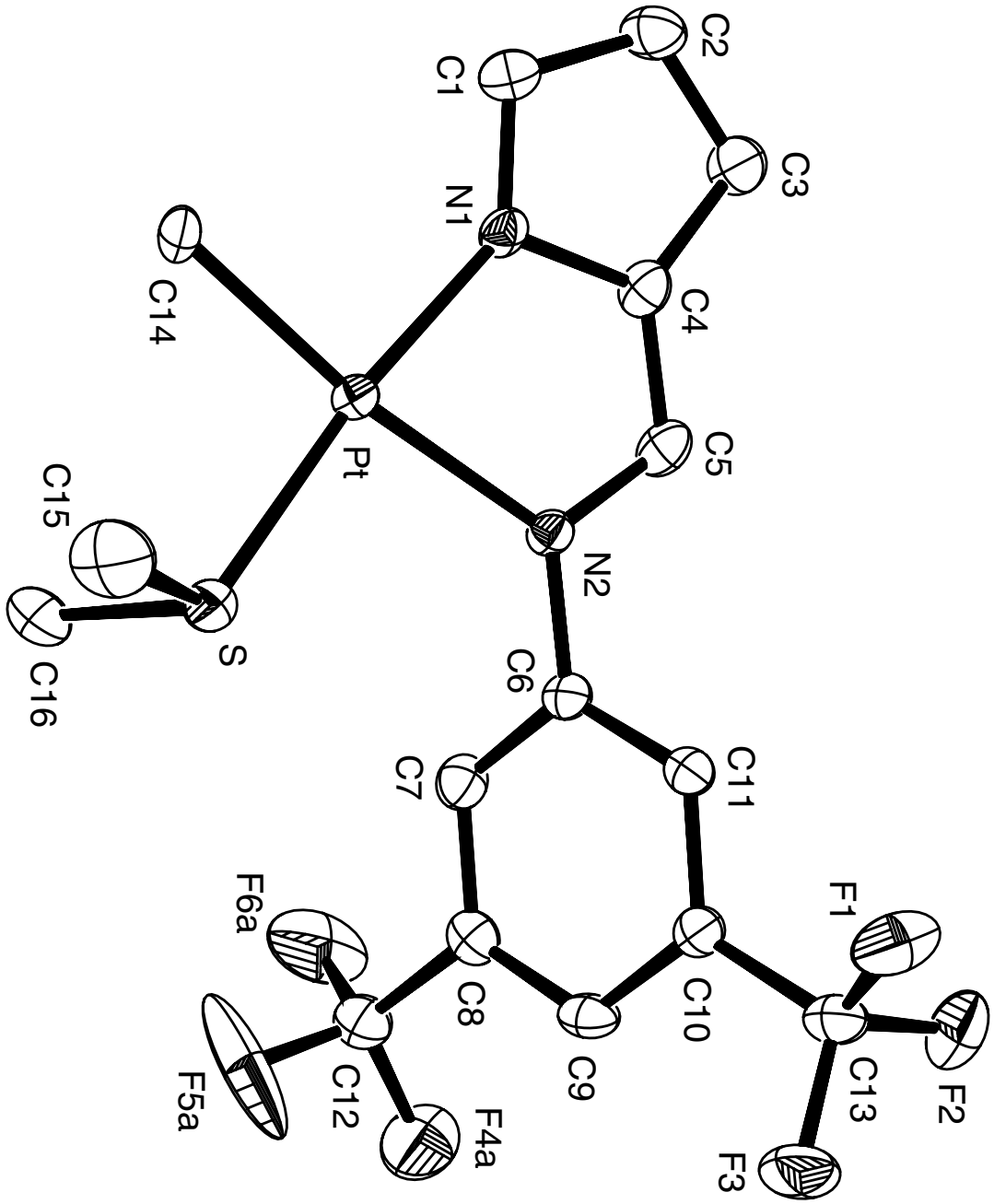


Figure 1. Labeled ORTEP-3[1] view of *cis*-**2c** with 60% probability ellipsoids, without hydrogens.

Table 1. Crystal Data and Structure Analysis Details for **2c**.

Empirical formula	$C_{16}H_{16}F_6N_2PtS$	
Formula weight	577.46	
Crystallization solvent	toluene	
Crystal shape	needle	
Crystal color	pale yellow	
Crystal size	0.05 x 0.05 x 0.35 mm	
Data Collection		
Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000 ccd	
Wavelength	0.71073 Å MoKα	
Data collection temperature	98 K	
Theta range for 4520 reflections used in lattice determination	2.3 to 28.4°	
Unit cell dimensions	a = 8.4470(9) Å	α= 90°
	b = 9.4655(10) Å	β= 92.254(2)°
	c = 22.508(2) Å	γ = 90°
Volume	1798.3(3) Å^3	
Z	4	
Crystal system	monoclinic	
Space group	$P2_1/c$ (# 14)	
Density (calculated)	2.133 g/cm^3	
F(000)	1096	
Theta range for data collection	2.33 to 28.50°	
Completeness to theta = 28.50°	94.8%	
Index ranges	$-10 \le h \le 11$, $-12 \le k \le 12$, $-30 \le l \le 30$	
Data collection scan type	ω scans at 5 fixed ϕ values	
Reflections collected	26572	
Independent reflections	4320 [R_{int}= 0.0707]	
Reflections > 2σ(I)	3356	
Average σ(I)/(net I)	0.0497	
Absorption coefficient	7.980 mm^{-1}	
Absorption correction	Integration	
Max. and min. transmission	0.745 and 0.232	
Reflections monitored for decay	first 100 scans recollected at end of runs	
Decay of standards	within counting statistics	
Structure Solution and Refinement		
Primary solution method	Patterson map	
Secondary solution method	difference map	
Hydrogen placement	calculated	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4320 / 0 / 251	
Treatment of hydrogen atoms	mixed	
Goodness-of-fit on F^2	1.211	
Final R indices [I>2σ(I), 3356 reflections]	R1 = 0.0296, wR2 = 0.0456	

Table 1. Crystal Data and Structure Analysis Details for **2c**.

R indices (all data)	R1 = 0.0447, wR2 = 0.0474
Type of weighting scheme used	sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.066
Average shift/error	0.002
Largest diff. peak and hole	2.34 and -0.96 $e \cdot Å^{-3}$

Table 1. Crystal Data and Structure Analysis Details for **2c**.

Programs Used

Cell refinement	Bruker SAINT v6.02
Data collection	Bruker SMART v5.606
Data reduction	Bruker SAINT v6.02
Structure solution	SHELXS-97 (Sheldrick, 1990)
Structure refinement	SHELXL-97 (Sheldrick, 1997)
Twin analysis	Bruker Gemini 1.02

Special Refinement Details

The crystals submitted for analysis were pale yellow rectangular plates that typically formed clusters radiating from a center point with incipient cracks along the long axis. Data were collected for a small clear fragment and a structural solution obtained. However the crystal was twinned by 180° rotation about the c^* axis, with one component a bit larger than the other. All reflections were fully or partially overlapped with the maximum separation of spots in reciprocal space being ~0.22 $Å^{-1}$. This twinning precluded adequate refinement either as a two-component twin or a single crystal with many data excluded. Both approaches produced models which could be refined only isotropically, with one carbon atom refining to a negative U_{iso}. Other specimens examined were also twinned. After extensive examination, a single pale yellow needle was found amidst the plates. This crystal subsequently proved to be only slightly twinned. One end of the crystal was trimmed off and the remainder was mounted on a glass fiber with Paratone-N oil. Five runs of data were collected with 15 second long, –0.30° wide ω–scans at five values of φ (0, 72, 144, 216, and 288°) with the detector 5 cm (nominal) distant at a θ of -28° using SMART v5.606. The initial cell for data reduction was calculated from 999 reflections chosen from throughout the data frames. During least-squares refinement of this cell, 176 reflections, primarily with distinctly non-integral indices and presumably from a twin, were thrown out. For data processing with SAINT v6.02, all defaults were used, except: a fixed box size of 1.8 x 1.8 x 0.7 was used, periodic orientation matrix updating was disabled, the instrument error was set to zero, no Laue class integration restraints were used, and for the post-integration global least squares refinement, no constraints were applied. The faces of the crystal were indexed, and a Gaussian face-indexed absorption correction was applied with XPREP v6.10. No decay correction was needed.

Two outlier reflections (0 0 2 and -1 1 2) were omitted from the final processed dataset; 918 of 27490 reflections were rejected, with 0 space group-absence violations and 13 inconsistent equivalents. Refinement of F^2 was against all reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement.

There is one molecule in the asymmetric unit. The conformation of the molecule is similar to those of the related compound **1c**. One of the CF_3 groups is disordered; it was modeled with one set of three anisotropic F atoms [occupancy 92.0(8)%] and one set of three isotropic F atoms [occupancy 8.0(8)%]. Hydrogen atoms were placed at calculated positions with U_{iso}'s set at 120% of the U_{eq}'s of the attached atoms; the methyl groups were allowed to rotate. The largest positive and negative excursions in the final difference map are 2.34 e·$Å^{-3}$ (0.06Å from Pt), 1.51 e·$Å^{-3}$ (0.98Å from Pt), and –0.96 e·$Å^{-3}$ (0.51Å from Pt). There are also 4 other peaks > 1 e·$Å^{-3}$ which are ~ 1Å from the Pt atom.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **2c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Pt	6801(1)	9123(1)	7624(1)	14(1)
S	4960(1)	8614(1)	8289(1)	20(1)
N1	8476(4)	9812(3)	7080(2)	15(1)
N2	8219(4)	10417(3)	8209(2)	14(1)
C1	8800(5)	9721(4)	6497(2)	19(1)
C2	10059(5)	10609(4)	6374(2)	23(1)
C3	10524(5)	11274(4)	6898(2)	22(1)
C4	9518(5)	10778(5)	7334(2)	18(1)
C5	9343(5)	11067(4)	7939(2)	19(1)
C6	8003(5)	10696(4)	8824(2)	14(1)
C7	7970(5)	9588(4)	9222(2)	19(1)
C8	7697(5)	9839(4)	9815(2)	17(1)
C9	7441(5)	11194(4)	10015(2)	18(1)
C10	7467(5)	12308(4)	9609(2)	16(1)
C11	7751(5)	12069(4)	9024(2)	14(1)
C12	7650(6)	8634(5)	10239(2)	23(1)
C13	7190(5)	13784(4)	9823(2)	21(1)
C14	5695(5)	7939(4)	6975(2)	22(1)
C15	3026(5)	8818(5)	7943(2)	33(1)
C16	4966(6)	6754(5)	8415(2)	31(1)
F1	6532(3)	14599(3)	9400(1)	31(1)
F2	8560(3)	14419(3)	9993(1)	32(1)
F3	6280(3)	13833(3)	10290(1)	35(1)
F4A[a]	8158(5)	8987(4)	10793(2)	47(1)
F5A[a]	6248(4)	8102(5)	10283(2)	74(2)
F6A[a]	8619(5)	7584(4)	10105(2)	53(1)
F4B[b]	8720(40)	8400(30)	10554(16)	19(9)
F5B[b]	7280(40)	7420(30)	9966(13)	19(9)
F6B[b]	6440(50)	8800(40)	10609(17)	35(11)

[a] Population: 0.920(8)
[b] Population: 0.080(8)
[c] U_{iso}

Table 3. Bond lengths [Å] for **2c**.

Pt-N1	2.016(3)	C9-C10	1.396(6)
Pt-C14	2.038(4)	C9-H9	0.9500
Pt-N2	2.132(3)	C10-C11	1.367(5)
Pt-S	2.2537(12)	C10-C13	1.499(6)
S-C16	1.783(4)	C11-H11	0.9500
S-C15	1.793(5)	C12-F4A	1.346(6)
N1-C1	1.354(5)	C12-F5A	1.294(6)
N1-C4	1.378(5)	C12-F6A	1.330(5)
N2-C5	1.302(5)	C12-F4B	1.15(3)
N2-C6	1.426(5)	C12-F5B	1.33(3)
C1-C2	1.392(6)	C12-F6B	1.35(4)
C1-H1	0.9500	C13-F3	1.327(5)
C2-C3	1.380(6)	C13-F1	1.331(5)
C2-H2	0.9500	C13-F2	1.346(5)
C3-C4	1.406(6)	C14-H14A	0.9800
C3-H3	0.9500	C14-H14B	0.9800
C4-C5	1.402(6)	C14-H14C	0.9800
C5-H5	0.9500	C15-H15A	0.9800
C6-C7	1.381(5)	C15-H15B	0.9800
C6-C11	1.394(5)	C15-H15C	0.9800
C7-C8	1.383(6)	C16-H16A	0.9800
C7-H7	0.9500	C16-H16B	0.9800
C8-C9	1.379(6)	C16-H16C	0.9800
C8-C12	1.488(6)		

Table 4. Bond angles [°] for **2c**.

N1-Pt-C14	93.19(16)	C11-C10-C9	120.8(4)
N1-Pt-N2	78.41(13)	C11-C10-C13	120.0(4)
C14-Pt-N2	171.55(16)	C9-C10-C13	119.2(4)
N1-Pt-S	172.90(10)	C10-C11-C6	120.0(4)
C14-Pt-S	92.84(13)	C10-C11-H11	120.0
N2-Pt-S	95.60(10)	C6-C11-H11	120.0
C16-S-C15	99.9(2)	F5A-C12-F6A	107.5(4)
C16-S-Pt	108.59(17)	F4B-C12-F5B	107(2)
C15-S-Pt	109.19(17)	F5A-C12-F4A	106.5(4)
C1-N1-C4	107.2(3)	F6A-C12-F4A	102.7(4)
C1-N1-Pt	137.9(3)	F4B-C12-F6B	104(2)
C4-N1-Pt	114.5(3)	F5B-C12-F6B	102(2)
C5-N2-C6	119.2(3)	F4B-C12-C8	120.3(15)
C5-N2-Pt	112.6(3)	F5A-C12-C8	113.3(4)
C6-N2-Pt	128.0(3)	F6A-C12-C8	113.3(4)
N1-C1-C2	109.8(4)	F5B-C12-C8	112.0(13)
N1-C1-H1	125.1	F4A-C12-C8	112.9(4)
C2-C1-H1	125.1	F6B-C12-C8	110.4(15)
C3-C2-C1	107.4(4)	F3-C13-F1	107.9(4)
C3-C2-H2	126.3	F3-C13-F2	106.1(4)
C1-C2-H2	126.3	F1-C13-F2	105.9(3)
C2-C3-C4	106.6(4)	F3-C13-C10	112.9(4)
C2-C3-H3	126.7	F1-C13-C10	112.1(4)
C4-C3-H3	126.7	F2-C13-C10	111.4(4)
N1-C4-C5	116.3(4)	Pt-C14-H14A	109.5
N1-C4-C3	108.9(4)	Pt-C14-H14B	109.5
C5-C4-C3	134.7(4)	H14A-C14-H14B	109.5
N2-C5-C4	117.9(4)	Pt-C14-H14C	109.5
N2-C5-H5	121.0	H14A-C14-H14C	109.5
C4-C5-H5	121.0	H14B-C14-H14C	109.5
C7-C6-C11	119.4(4)	S-C15-H15A	109.5
C7-C6-N2	119.7(4)	S-C15-H15B	109.5
C11-C6-N2	120.8(3)	H15A-C15-H15B	109.5
C6-C7-C8	120.3(4)	S-C15-H15C	109.5
C6-C7-H7	119.8	H15A-C15-H15C	109.5
C8-C7-H7	119.8	H15B-C15-H15C	109.5
C9-C8-C7	120.5(4)	S-C16-H16A	109.5
C9-C8-C12	119.7(4)	S-C16-H16B	109.5
C7-C8-C12	119.8(4)	H16A-C16-H16B	109.5
C8-C9-C10	118.9(4)	S-C16-H16C	109.5
C8-C9-H9	120.6	H16A-C16-H16C	109.5
C10-C9-H9	120.6	H16B-C16-H16C	109.5

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **2c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt	161(1)	140(1)	121(1)	-11(1)	0(1)	-11(1)
S	199(6)	230(6)	167(6)	-29(5)	24(5)	-53(5)
N1	161(19)	131(17)	160(20)	-41(15)	26(16)	15(15)
N2	117(19)	153(17)	147(19)	-30(14)	21(15)	-2(14)
C1	200(30)	230(20)	160(20)	-14(19)	-10(20)	23(19)
C2	200(20)	310(30)	180(20)	-10(20)	40(20)	0(20)
C3	160(20)	280(30)	230(30)	-30(20)	30(20)	-37(18)
C4	120(20)	200(20)	210(20)	-30(20)	-12(18)	-7(19)
C5	150(20)	220(20)	190(20)	-50(20)	-38(18)	-4(19)
C6	100(20)	190(20)	130(20)	-10(18)	-18(17)	-13(17)
C7	200(30)	170(20)	190(30)	0(18)	-20(20)	-6(18)
C8	130(20)	200(20)	190(30)	20(19)	-5(19)	2(18)
C9	170(20)	270(30)	110(20)	-2(19)	-3(18)	-3(18)
C10	110(20)	190(20)	180(20)	-33(19)	18(18)	-15(18)
C11	110(20)	190(20)	130(20)	14(18)	-19(18)	-17(17)
C12	290(30)	230(20)	190(30)	20(20)	10(20)	-10(20)
C13	220(30)	250(30)	170(20)	-17(19)	50(20)	7(19)
C14	280(30)	190(20)	170(20)	1(19)	-30(20)	-120(20)
C15	170(30)	480(30)	330(30)	-30(20)	20(20)	10(20)
C16	450(30)	280(30)	220(30)	40(20)	80(20)	-100(20)
F1	459(18)	267(14)	192(15)	-16(12)	-40(13)	174(13)
F2	324(16)	257(15)	382(18)	-97(13)	-33(13)	-48(12)
F3	484(19)	295(17)	303(17)	-35(13)	231(14)	63(13)
F4A	840(30)	340(20)	232(19)	83(18)	-84(19)	-40(20)
F5A	230(20)	910(40)	1070(40)	760(30)	-210(20)	-270(20)
F6A	810(30)	340(20)	450(20)	219(18)	230(20)	270(20)

Table 6. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for **2c**.

	x	y	z	U_{iso}
H1	825	914	621	23
H2	1052	1073	600	28
H3	1136	1194	695	27
H5	1002	1172	815	22
H7	814	865	909	23
H9	725	1137	1042	22
H11	778	1284	875	17
H14A	498	726	716	26
H14B	649	743	675	26
H14C	508	856	670	26
H15A	222	863	823	39
H15B	290	815	761	39
H15C	290	979	779	39
H16A	596	648	862	37
H16B	486	626	803	37
H16C	408	650	866	37

Table 6. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for **2c**.

0.0165	0.0143	0.0114	Pt
0.0279	0.0162	0.0155	S
0.0194	0.0167	0.0095	N1
0.0181	0.0128	0.0106	N2
0.0244	0.0186	0.0153	C1
0.0312	0.0227	0.0153	C2
0.0311	0.0215	0.0143	C3
0.0233	0.0182	0.0117	C4
0.0259	0.0188	0.0113	C5
0.0189	0.0142	0.0088	C6
0.0226	0.0177	0.0169	C7
0.0219	0.0180	0.0124	C8
0.0274	0.0167	0.0111	C9
0.0221	0.0150	0.0108	C10
0.0195	0.0136	0.0096	C11
0.0289	0.0239	0.0178	C12
0.0256	0.0238	0.0137	C13
0.0372	0.0174	0.0100	C14
0.0481	0.0328	0.0171	C15
0.0495	0.0291	0.0150	C16
0.0572	0.0190	0.0160	F1
0.0439	0.0349	0.0179	F2
0.0622	0.0317	0.0125	F3
0.0867	0.0373	0.0181	F4A
0.1847	0.0249	0.0121	F5A
0.1049	0.0384	0.0156	F6A

References

(1)Farrugia, L. J. *J. Appl. Crys.* **1997**, *30*, 565.